
Vortex-impurity interactions in two-dimensional quantum fluids

A thesis submitted to the School of Engineering, Mathematics
and Physics at the University of East Anglia in partial
fulfilment of the requirements for the degree of Doctor of
Philosophy

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January/2026

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Abstract

This thesis investigates the behaviour of a quantum impurity coupled to a Bose–Einstein condensate. The condensate dynamics are described by the Gross–Pitaevskii equation, while the impurity is modelled by a coupled Schrödinger equation, forming a Gross–Clark-system. The work focuses on impurity localisation, vortex structure, and the dynamical consequences of impurity-condensate coupling in effectively two-dimensional geometries.

The thesis begins by establishing the Gross–Pitaevskii model and its dimensionless formulation, together with the structure and stability of quantised vortices. Both numerical and approximate analytical descriptions of vortex profiles are developed and used throughout the thesis. The localisation of impurities is then examined in a range of static settings, including idealised trapping potentials and vortex cores, revealing how condensate density depletion can generate effective confinement for the impurity.

Self-consistent impurity-vortex bound states are obtained by solving coupled stationary equations. The spectrum of localised impurity states is analysed, and the dependence of localisation on interaction parameters and angular momentum is characterised. These static results provide the foundation for subsequent dynamical studies.

Real-time simulations are used to investigate the stability of impurity-bound configurations. For singly quantised vortices, impurity ground states are shown to

be dynamically robust, while excited impurity states relax under time evolution despite remaining localised. A quantitative overlap measure is introduced to characterise the dynamical stability of impurity states. The thesis then examines multiply quantised vortices, demonstrating that impurity coupling can modify vortex dynamics and, in certain cases, suppress intrinsic instabilities.

Overall, this work provides a systematic analysis of impurity localisation and impurity–vortex interactions in Bose-Einstein condensates, combining theoretical modelling, numerical methods, and dynamical simulations to clarify the role of impurities in coupled quantum fluids.

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Acknowledgements

I would like to express my sincere gratitude to my supervisor, Dr. Davide Proment, for his guidance, support, and patience throughout my PhD. His advice, encouragement, and academic insight were essential to the completion of this thesis.

I am also very grateful to Dr. Alberto Villosi for his support and valuable discussions during my research. His help and feedback contributed greatly to the development of this work.

I would like to express my deepest gratitude to my parents for their love, prayers, and constant support throughout this journey. I am also sincerely thankful to my brothers and sisters for their care and encouragement, which made me feel supported at all times. Special thanks go to my brother Shaker for his exceptional support during the first year of my PhD. His presence, sacrifices, and encouragement played an important role in helping me continue this journey.

I am deeply grateful to my husband for his constant support, patience, and understanding. He stood by me during the most challenging moments, shared responsibilities, and supported me without hesitation. This achievement would not have been possible without him.

To my son Raed, my eldest, thank you for your maturity, responsibility, and understanding beyond your years. You were a source of strength and reassurance

throughout this journey.

To my daughter Sarah, my right hand, thank you for always helping me, taking responsibility, and supporting me in countless ways. Your support made many difficult days easier.

To my daughter Hoor, thank you for the joy, laughter, and happiness you brought into our lives. Your energy, playful movements, sweet messages, and endless questions filled our home with life and warmth.

To my son Mansour, the soul of our home, you came into my life in the first year of my PhD and truly brought smiles, laughter, and happiness to our family. You were a constant reminder of joy and hope throughout this journey.

This thesis is not only the result of years of academic work, but also a reflection of the patience, support, and love of my family and mentors, without whom this journey would not have been possible.

Introduction

1.1 Bose-Einstein condensation and superfluidity

A Bose-Einstein condensate (BEC) is a state of matter in which a macroscopic number of bosons occupy the same single-particle quantum state. This regime is typically realised either in dilute atomic gases cooled to temperatures near absolute zero or in systems at very high densities, such as neutron stars, where quantum statistics dominate the thermodynamic behaviour of the fluid [46, 47, 16]. In these conditions, quantum coherence extends over length scales that are large compared with the interparticle spacing, so that interference and phase coherence become observable at macroscopic scales.

The first dilute-gas BECs were created in the mid-1990s using alkali atoms confined in magnetic or optical traps and cooled by a combination of laser and evaporative cooling [36, 14]. These experiments confirmed long-standing theoretical predictions and opened a versatile platform for exploring quantum many-body physics under highly controllable conditions. In particular, ultracold atomic gases allow experimental access to tunable interaction strengths, dimensionality, disorder and trapping geometries, making them ideal systems for testing condensed-matter concepts in a clean and flexible setting [46, 47, 16].

Bose-Einstein condensation is closely connected to, but not identical with, superfluidity. Superfluidity refers to the ability of a fluid to support frictionless flow below a critical velocity and to sustain quantised vortices. It was first

identified in liquid helium, where the transition to the superfluid phase is accompanied by a sharp change in thermodynamic properties and transport coefficients [47, 38]. In dilute atomic gases, BECs generally exhibit superfluid properties, and the condensate wavefunction provides a convenient order parameter for describing both the condensed and superfluid phases. Not every condensate is necessarily superfluid and not every superfluid arises from conventional Bose-Einstein condensation, but in weakly interacting dilute gases the two phenomena are intimately linked [38, 47].

For weakly interacting bosons at low temperatures, the condensate order parameter is accurately described by the Gross-Pitaevskii equation (GPE), a nonlinear Schrödinger equation derived within a mean-field framework [46, 47, 53, 8]. The GPE has become the standard theoretical model for dilute BECs and provides the basis for much of the analysis developed in this thesis, including the description of quantised vortices and the coupling between a condensate and an impurity field.

1.2 Vortices in quantum fluids

One of the most striking manifestations of superfluidity is the existence of quantised vortices. Quantum vortices are topological defects of the condensate wavefunction in which the density is strongly depleted at the core and the phase winds by an integer multiple of 2π around a closed path. This structure enforces quantisation of circulation: in contrast to classical fluids, where vortices can carry arbitrary circulation, the circulation in a quantum vortex is fixed by the requirement that the condensate wavefunction remain single-valued [19, 51].

Quantised vortices were first observed in superfluid helium and later in trapped dilute BECs [14]. In atomic condensates, vortices can be generated by rotating the trap, by stirring the condensate with focused laser beams, or by phase-imprinting techniques [41, 40, 19]. Subsequent experiments have

demonstrated vortex lattices, vortex dipoles and more complex configurations, firmly establishing quantised vortices as key signatures of superfluid behaviour in quantum fluids [14, 19].

Within the GPE framework, a vortex corresponds to a stationary, localised disturbance of the condensate wavefunction. The size of the vortex core is set by the healing length, which characterises the balance between kinetic and interaction energies in the fluid [46, 16]. Collections of vortices in a rotating condensate can form ordered lattices, while their interactions, reconnections and decay processes underpin the phenomenon of quantum turbulence [19, 63]. Understanding vortex dynamics is therefore central to the broader study of superfluid hydrodynamics, quantum phase transitions and the stability of excited states in quantum fluids.

1.3 Impurities in quantum fluids

Impurities provide a powerful probe of superfluid properties and quantum coherence. In dilute BECs, an “impurity” may correspond to a distinguishable atomic species, a different internal state of the same atom, or an externally imposed localised potential created, for example, by a tightly focused laser beam [10, 43, 57]. Depending on the setup, impurities can be static, mobile or externally driven, and can interact repulsively or attractively with the host condensate.

The dynamics of impurities in superfluids have been studied since Landau’s original argument for a critical velocity below which a particle can move without creating excitations [37]. In ultracold gases, controlled experiments have observed regimes where impurities propagate essentially undamped, as well as regimes where they emit phonons, shed vortices and generate turbulence once a critical velocity is exceeded [67, 31, 61]. At the microscopic level, a mobile impurity can become dressed by excitations of the host fluid, forming a

Bose polaron whose effective mass, energy and coherence properties can be measured experimentally [34, 33, 28, 25].

The presence of quantised vortices introduces additional richness. The vortex core is a region of suppressed condensate density and therefore acts as an effective potential well for an impurity. Impurities can become trapped in vortex cores, modify the local density and phase structure, and in turn alter the dynamical behaviour of the vortex. Theoretical and experimental studies have shown that vortex-trapped impurities can lead to localised bound states, affect vortex trajectories and enable impurity-mediated interactions between vortices [5, 50, 7]. More generally, impurities and vortices can form composite excitations in which the impurity dressing endows the vortex with an effective inertial mass, enabling dynamical processes not present in an otherwise massless vortex fluid [63, 13, 23, 17, 49].

Many of these phenomena can be modelled using coupled mean-field equations that extend the GPE to include an impurity degree of freedom. In this thesis we employ the Gross-Clark framework, which couples the Gross-Pitaevskii equation for the condensate to a Schrödinger equation for the impurity and captures the reciprocal interaction between the two fields in a quasi-two-dimensional geometry [53, 7].

1.4 Scope and structure of this thesis

The central aim of this thesis is to investigate the behaviour of quantum impurity embedded in a Bose-Einstein condensate, with particular emphasis on self-localisation phenomena and on the interplay between impurity and quantised vortices. We work within the Gross-Pitaevskii and Gross-Clark mean-field frameworks, focusing primarily on quasi-two-dimensional geometries relevant to experiments with trapped ultracold gases [46, 53, 7].

Part I introduces the theoretical models used throughout the thesis. Chapter 2

presents the Gross-Pitaevskii equation, including its mean-field derivation, non-dimensionalisation, conserved quantities and hydrodynamic formulation, with particular attention to vortex solutions [46, 47, 16]. Chapter 3 reviews the linear Schrödinger equation in one and two dimensions and discusses model potentials relevant for impurity confinement. Chapter 4 introduces the Gross-Clark model, its dimensional reduction to a quasi-two-dimensional geometry, and its numerical implementation via imaginary-time and real-time propagation schemes.

Part II contains the original results. Chapter 5 studies the self-localisation of a single impurity field in a homogeneous condensate, combining numerical simulations with a variational analysis to determine the threshold for localisation and to map the associated phase diagram. Chapter 6 investigates the eigenstates of an impurity trapped in the core of a quantised vortex in two dimensions, using an iterative numerical scheme to solve the coupled condensate-impurity problem and to characterise the back-action of the impurity on the vortex structure. Chapter 7 examines how a localised impurity affects the dynamical stability of both single and multiply quantized vortices, demonstrating regimes in which the impurity can suppress the splitting instability and thereby stabilise the condensate.

Part III summarises the main conclusions and outlines possible directions for future work, including extensions to fully three-dimensional geometries, finite-temperature effects, and systems involving multiple impurities or more complex trapping configurations.

Part I

Theoretical Models

The Gross–Pitaevskii Model

This chapter establishes the theoretical framework used to describe the dynamics of dilute Bose–Einstein condensates (BECs) within the Gross–Pitaevskii equation (GPE). We first derive the GPE as a mean-field model for a weakly interacting Bose gas and the quasi-two-dimensional reduction appropriate to strongly confined geometries. Then introduce the main conserved quantities, the dimensionless form, and the hydrodynamic (Madelung) formulation, which provides a fluid-dynamical interpretation of the condensate.

We then explore the structure of quantized vortices, which are topological excitations supported by the GPE, and analyse their stationary profiles in the homogeneous two-dimensional limit. In particular, we derive the radial vortex equation and present Padé approximations for singly and doubly quantized vortices, which will be used as initial conditions and reference states in later simulations. These results provide the background against which impurity–vortex interaction models and coupled dynamics will be developed in subsequent chapters.

2.1 Mean-Field Derivation

The Gross–Pitaevskii equation (GPE) provides a mean-field framework for describing the dynamics of a dilute Bose–Einstein condensate (BEC) in the

limit of zero temperature. The key assumption is that all bosons occupy the same quantum state, allowing the many-body wavefunction to be approximated by a product of identical single-particle wavefunctions [46, 47].

We consider a system of N identical bosons of mass m confined in an external potential $V_{\text{ext}}(\mathbf{r})$, and interacting via a two-body potential $V(\mathbf{r}_i - \mathbf{r}_j)$. The full many-body Hamiltonian operator is given by

$$\hat{H} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) \right) + \sum_{1 \leq i < j \leq N} V(\mathbf{r}_i - \mathbf{r}_j). \quad (2.1.1)$$

In the dilute limit, where the average interparticle spacing is much larger than the range of interatomic forces, the interaction potential can be well approximated by a contact pseudopotential:

$$V(\mathbf{r}) = g \delta(\mathbf{r}), \quad \text{with} \quad g = \frac{4\pi\hbar^2 a_s}{m}, \quad (2.1.2)$$

and a_s is the s -wave scattering length [47, 38].

Within the Hartree mean-field approximation, the many-body wavefunction is represented by a product of identical single-particle states. This motivates the introduction of a condensate wavefunction $\psi_{3D}(\mathbf{r}, t)$ such that

$$\int |\psi_{3D}(\mathbf{r}, t)|^2 d\mathbf{r} = N, \quad (2.1.3)$$

so that $|\psi_{3D}(\mathbf{r}, t)|^2$ is the particle density of the condensate. Evaluating the expectation value of the Hamiltonian (2.1.1) in a corresponding Hartree product state, and using the contact form (2.1.2) for the interaction, leads to the Gross–Pitaevskii energy functional

$$E_{GP} = \int \left[\frac{\hbar^2}{2m} |\nabla \psi_{3D}|^2 + V_{\text{ext}} |\psi_{3D}|^2 + \frac{g}{2} |\psi_{3D}|^4 \right] d\mathbf{r}. \quad (2.1.4)$$

We denote the Gross–Pitaevskii energy by the functional E_{GP} in order to

distinguish it from the impurity energy eigenvalues E introduced in later chapters. The ground state of the system is obtained by minimizing E_{GP} subject to the normalization constraint (2.1.3). Introducing a Lagrange multiplier μ (the chemical potential) leads to the Euler–Lagrange condition

$$\frac{\delta}{\delta\psi_{3D}^*} \left(E_{GP} - \mu \int |\psi_{3D}|^2 d\mathbf{r} \right) = 0, \quad (2.1.5)$$

which yields the time-independent Gross–Pitaevskii equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\psi_{3D}(\mathbf{r})|^2 \right) \psi_{3D}(\mathbf{r}) = \mu\psi_{3D}(\mathbf{r}). \quad (2.1.6)$$

Allowing the condensate wavefunction to evolve dynamically and applying a time-dependent variational principle [30, 16] leads to the time-dependent Gross–Pitaevskii equation

$$i\hbar \frac{\partial\psi_{3D}(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\psi_{3D}(\mathbf{r}, t)|^2 \right) \psi_{3D}(\mathbf{r}, t) \quad (2.1.7)$$

with the normalization (2.1.3) is preserved by the dynamics.

The GPE is a nonlinear Schrödinger equation that captures essential features of dilute condensates, including superfluidity and the formation of quantized vortices. It forms the basis for much of the theoretical and numerical work on BECs at ultracold temperatures, as will be shown in the following sections.

2.2 Two-Dimensional Limit and Quasi-2D Confinement

The dimensionless Gross–Pitaevskii equation derived previously is applicable to a three-dimensional (3D) Bose–Einstein condensate (BEC). In this thesis, we focus on a regime where the system is effectively two-dimensional (2D), consistent with the geometry employed in subsequent simulations and impurity–coupling models

[22, 27].

A quasi-2D approximation becomes valid when the condensate is tightly confined along one spatial direction, typically the z -axis, by a strong trapping potential. We assume the potential to be harmonic, of the form

$$V_{\text{ext}}(z) = \frac{1}{2}m\omega_z^2 z^2, \quad (2.2.1)$$

where ω_z is the trap frequency. If the confinement energy satisfies $\hbar\omega_z \gg \mu$, the motion along z is frozen into the ground state of the harmonic oscillator, and the condensate behaves as a two-dimensional fluid [27, 54].

In this regime, the condensate wavefunction factorizes into an in-plane and an axial part:

$$\psi_{3D}(x, y, z, t) = \psi_{2D}(x, y, t) \phi_0(z), \quad (2.2.2)$$

where $\psi_{2D}(x, y, t)$ is the effective 2D condensate wavefunction and $\phi_0(z)$ is the ground-state harmonic oscillator wavefunction,

$$\phi_0(z) = \frac{1}{\pi^{1/4} a_z^{1/2}} e^{-z^2/(2a_z^2)}, \quad a_z = \sqrt{\frac{\hbar}{m\omega_z}}, \quad (2.2.3)$$

with a_z the harmonic oscillator length associated with the confinement along the z -axis. The axial mode is normalized to unity, $\int |\phi_0(z)|^2 dz = 1$, so that the 3D normalization $\int |\psi_{3D}|^2 d^3\mathbf{r} = N$ reduces to

$$\int |\psi_{2D}(x, y)|^2 dx dy = N. \quad (2.2.4)$$

The 3D interaction energy is

$$E_{\text{int-GP}} = \frac{g}{2} \int |\psi_{3D}|^4 d^3\mathbf{r}. \quad (2.2.5)$$

Substituting the factorized form and integrating over z gives

$$E_{\text{int-GP}} = \frac{g}{2\sqrt{2\pi}a_z} \int |\psi_{2D}(x, y)|^4 dx dy. \quad (2.2.6)$$

This has the same structure as a 2D interaction with coupling constant

$$g_{2D} = \frac{g}{\sqrt{2\pi}a_z} = \sqrt{8\pi} \frac{\hbar^2 a_s}{ma_z}. \quad (2.2.7)$$

From this point on, unless explicitly stated otherwise, ψ denotes the effective two-dimensional condensate wavefunction ψ_{2D} .

Thus, integrating out the frozen z -dimension renormalizes the 3D coupling g to an effective 2D coupling g_{2D} that depends on the confinement length a_z . This quasi-2D limit is widely used in theoretical and experimental studies of flat or pancake-shaped BECs and provides the framework for the models developed in this thesis.

2.3 Conserved Quantities

The Gross–Pitaevskii equation (GPE) possesses several conservation laws that arise from the symmetries of the system. These conserved quantities include the total number of atoms, total energy, and momentum. Their conservation reflects underlying symmetries in the system and serves as a useful check in numerical simulations. Specifically:

- The **particle number** is always conserved.
- The **total energy** is conserved if the external potential is time-independent.
- The **linear momentum** is conserved if the external potential is constant or periodic.
- The **angular momentum** is conserved if the external potential is rotationally symmetric.

1. Particle number: The total number of atoms

$$N = \int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} \quad (2.3.1)$$

is conserved. Taking the time derivative gives:

$$\frac{dN}{dt} = \int \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) d\mathbf{r} \quad (2.3.2)$$

Substituting (2.1.7) and its complex conjugate into (2.3.2), and after simplification

$$\frac{dN}{dt} = 0.$$

2. Energy: The total energy is

$$E_{GP} = \int \left[\frac{\hbar^2}{2m} |\nabla \psi|^2 + V_{\text{ext}} |\psi|^2 + \frac{g}{2} |\psi|^4 \right] d\mathbf{r} \quad (2.3.3)$$

Differentiating with respect to time gives

$$\frac{dE_{GP}}{dt} = \int \left[\frac{\hbar^2}{2m} \left(\nabla \psi^* \cdot \nabla \frac{\partial \psi}{\partial t} + \nabla \psi \cdot \nabla \frac{\partial \psi^*}{\partial t} \right) + V_{\text{ext}} \frac{\partial}{\partial t} |\psi|^2 + g |\psi|^2 \text{Re} \left(\psi^* \frac{\partial \psi}{\partial t} \right) \right] d\mathbf{r}. \quad (2.3.4)$$

Substituting (2.1.7) into this expression and simplifying yields

$$\frac{dE_{GP}}{dt} = \int (\partial_t V_{\text{ext}}) |\psi|^2 d\mathbf{r}. \quad (2.3.5)$$

Therefore, if V_{ext} is time-independent, $\partial_t V_{\text{ext}} = 0$ and $dE_{GP}/dt = 0$, the total energy is conserved for a time-independent external potential.

3. Linear momentum. The linear momentum of the condensate is obtained from the quantum mechanical momentum operator $-i\hbar\nabla$ applied to the condensate wavefunction. The expectation value is

$$\mathbf{P} = \int \psi^* (-i\hbar\nabla) \psi d\mathbf{r} = -\frac{i\hbar}{2} \int (\psi^* \nabla \psi - \psi \nabla \psi^*) d\mathbf{r}. \quad (2.3.6)$$

Taking the time derivative and substituting (2.1.7) gives

$$\frac{d\mathbf{P}}{dt} = - \int (\nabla V_{\text{ext}}) |\psi|^2 d\mathbf{r}. \quad (2.3.7)$$

This shows that the rate of change of momentum is equal to the net force generated by the external potential, as expected from Ehrenfest’s theorem. Therefore, $\mathbf{P}$ is conserved if V_{ext} is constant, so that the integral of ∇V_{ext} vanishes.

4. Angular momentum. In two-dimensional or cylindrically symmetric systems, the relevant conserved quantity is the angular momentum about the z -axis. It is obtained from the operator $\hat{L}_z = -i\hbar\partial_\theta$ in polar coordinates. The expectation value is

$$L_z(t) = \int \psi^*(x, y, t) (-i\hbar\partial_\theta) \psi(x, y, t) d^2\mathbf{r} = -\frac{i\hbar}{2} \int \left(\psi^* \frac{\partial\psi}{\partial\theta} - \psi \frac{\partial\psi^*}{\partial\theta} \right) d^2\mathbf{r}. \quad (2.3.8)$$

We focus on the z -component because the condensate is effectively confined to the x - y plane, so rotations around z are the only symmetry operations that apply.

Taking the time derivative and substituting the GPE yields

$$\frac{dL_z}{dt} = - \int \left(\frac{\partial V_{\text{ext}}}{\partial\theta} \right) |\psi|^2 d^2\mathbf{r}. \quad (2.3.9)$$

If V_{ext} has rotational symmetry, then $\partial V_{\text{ext}}/\partial\theta = 0$, which implies

$$\frac{dL_z}{dt} = 0. \quad (2.3.10)$$

Thus the angular momentum about the z -axis is conserved whenever the external potential is rotationally symmetric [47].

2.4 Dimensionless Form and Scaling Units

To simplify the Gross–Pitaevskii equation (GPE), we adopt a dimensionless formulation based on the natural units of a homogeneous Bose–Einstein condensate (BEC).

For a three-dimensional, untrapped BEC of bulk density ρ_{3D} , the chemical potential follows from the interaction energy per particle:

$$\mu = g \rho_{3D}. \quad (2.4.1)$$

where g is the interaction strength defined in Eq. (2.1.2) [46, 47]. The natural unit of length in this system is the healing length,

$$\xi = \sqrt{\frac{\hbar^2}{2m\mu}}, \quad (2.4.2)$$

which is obtained by balancing kinetic and interaction energies and sets the scale over which the condensate recovers from density perturbations. The corresponding characteristic time scale is set by the reciprocal of the chemical potential,

$$t_\mu = \frac{\hbar}{\mu}. \quad (2.4.3)$$

We now introduce rescaled dimensionless variables,

$$\tilde{\mathbf{r}} = \frac{\mathbf{r}}{\xi}, \quad \tilde{t} = \frac{t}{t_\mu}, \quad \tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t}) = \frac{\psi(\mathbf{r}, t)}{\sqrt{\rho_{3D}}}. \quad (2.4.4)$$

This choice ensures that the condensate density $|\tilde{\psi}|^2$ is of order unity in the bulk.

Under this scaling,

$$\frac{\partial}{\partial t} = \frac{1}{t_\mu} \frac{\partial}{\partial \tilde{t}}, \quad \nabla^2 = \frac{1}{\xi^2} \tilde{\nabla}^2. \quad (2.4.5)$$

To obtain the dimensionless form used throughout this thesis, we factor out the

trivial phase associated with the chemical potential by writing

$$\psi(\mathbf{r}, t) = \sqrt{\rho_{3D}} \tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t}) e^{-i\mu t/\hbar} \quad (2.4.6)$$

Substituting this expression, together with Eqs. (2.4.4) and (2.4.5) into (2.1.7) yields

$$i \frac{\partial \tilde{\psi}}{\partial \tilde{t}} = - \left(\frac{\hbar^2}{2m\mu\xi^2} \right) \tilde{\nabla}^2 \tilde{\psi} + \left(\frac{g \rho_{3D}}{\mu} \right) |\tilde{\psi}|^2 \tilde{\psi} - \tilde{\psi}. \quad (2.4.7)$$

Using the identities (2.4.1) and (2.4.2), we have $g \rho_{3D}/\mu = 1$ and $\hbar^2/(2m\mu\xi^2) = 1$, and therefore obtain the dimensionless Gross–Pitaevskii equation

$$i \frac{\partial \tilde{\psi}}{\partial \tilde{t}} = - \tilde{\nabla}^2 \tilde{\psi} + |\tilde{\psi}|^2 \tilde{\psi} - \tilde{\psi}. \quad (2.4.8)$$

Here, the nonlinear term $|\tilde{\psi}|^2 \tilde{\psi}$ represents the rescaled interaction energy, while the linear term $-\tilde{\psi}$ accounts for the background chemical potential [47, 16, 52]. For notational simplicity, we henceforth drop the tilde and denote the dimensionless condensate wavefunction again by ψ .

2.5 Madelung Transformation: Hydrodynamic Form of the GPE

For clarity, we work in the dimensionless units introduced in Sec. 2.4 and consider a homogeneous condensate without external potential. In these units, the time-dependent Gross–Pitaevskii equation (GPE) reads

$$i \frac{\partial \psi}{\partial t} = - \nabla^2 \psi + |\psi|^2 \psi - \psi. \quad (2.5.1)$$

The GPE can be recast in a hydrodynamic form through the Madelung transformation, which expresses the complex condensate wavefunction in terms

of a real-valued density and phase,

$$\psi(\mathbf{r}, t) = \sqrt{\rho(\mathbf{r}, t)} e^{iS(\mathbf{r}, t)}, \quad (2.5.2)$$

where $\rho = |\psi|^2$ is the condensate density and S is the phase. This decomposition allows the condensate to be interpreted as a compressible, inviscid, irrotational (barotropic) quantum fluid.

Substituting Eq. (2.5.2) into Eq. (2.5.1) and separating real and imaginary parts yields two coupled fluid-like equations:

1. Continuity equation (mass conservation):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (2.5.3)$$

where the superfluid velocity is

$$\mathbf{v} = \nabla S. \quad (2.5.4)$$

2. Quantum Euler equation:

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla \left(\frac{\mathbf{v}^2}{2} + \rho - \frac{1}{2} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right). \quad (2.5.5)$$

The final term, often called the quantum pressure, is absent in classical hydrodynamics and is essential for describing features such as vortex-core structure and dispersive (soliton-like) excitations.

Equations (2.5.3)–(2.5.5) show that the GPE describes an inviscid, irrotational, compressible fluid. This hydrodynamic picture is particularly useful when analysing the dynamics of quantized vortices and sound-like excitations.

Because the velocity field is given by $\mathbf{v} = \nabla S$, it is irrotational, $\nabla \times \mathbf{v} = \mathbf{0}$, everywhere that S is well defined. Singularities arise at points where the

condensate density vanishes, $\rho(\mathbf{r}, t) = 0$, since the phase of ψ is undefined there. In two dimensions, the zeros of ψ correspond to vortex cores. Around any closed loop encircling such a core, single-valuedness of the wavefunction requires the phase to wind by an integer multiple of 2π ,

$$\Delta S = 2\pi n, \quad n \in \mathbb{Z},$$

which leads to quantized circulation,

$$\oint \mathbf{v} \cdot d\boldsymbol{\ell} = 2\pi n. \quad (2.5.6)$$

This circulation quantization is the defining feature of quantized vorticity in superfluids and will be explored in more detail in the next section.

2.6 Vortices

2.6.1 Formation, Quantization, and Significance

Quantized vortices are topological defects of the condensate phase in Bose–Einstein condensates (BECs). Because the wavefunction is single-valued, the phase S changes by an integer multiple of 2π around any closed loop C encircling a vortex [20]. Using $\mathbf{v} = \nabla S$ in the dimensionless units introduced above and the definition of circulation gives

$$\Gamma \equiv \oint_C \mathbf{v} \cdot d\boldsymbol{\ell} = \oint_C \nabla S \cdot d\boldsymbol{\ell} = 2\pi s, \quad s \in \mathbb{Z}, \quad (2.6.1)$$

Here s is the winding number (topological charge). In two dimensions, the velocity field of an isolated vortex is

$$\mathbf{v}(r) = \frac{s}{r} \hat{\boldsymbol{\theta}}$$

in dimensionless units.

At the vortex core the phase is undefined. To prevent a divergence of the kinetic energy density, which scales as $|\nabla S|^2 \sim 1/r^2$, the amplitude must vanish so that $|\psi(r)| \rightarrow 0$ as $r \rightarrow 0$. The density then recovers to the bulk value over the healing length ξ [46, 47].

Vortices play a central role in superfluid dynamics: they determine critical velocities, mediate quantum turbulence, and can act as trapping sites for impurities [19, 52]. Experimentally, they are generated by rotating the condensate, stirring it with a laser beam, or by optical phase imprinting [41, 40]. In simulations, vortices are introduced by imposing the corresponding phase winding.

The simplest vortex is singly quantized ($|s| = \pm 1$) with a 2π phase winding. Multiply quantized vortices ($|s| > 1$) are typically unstable because the kinetic energy scales as s^2 , they therefore tend to split into $|s|$ singly quantized vortices to minimise the total energy [19].

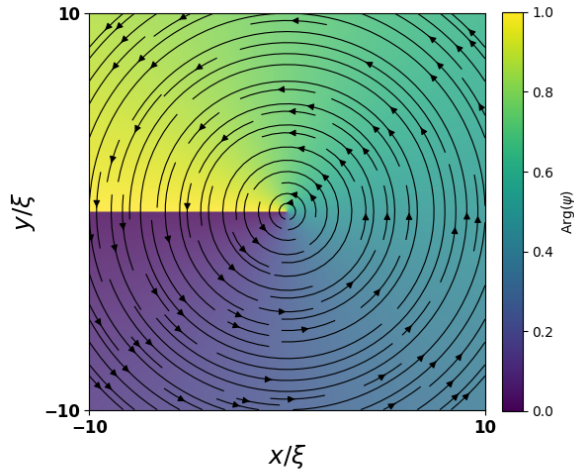


Figure 2.6.1: Velocity field (arrows) and condensate density (colour map) for a singly quantized ($s = 1$) 2D vortex. The velocity circulates as $\mathbf{v} = \hat{\boldsymbol{\theta}}/r$ and the density vanishes at the core, recovering over the healing length ξ . The circulation around any loop enclosing the core is quantized, $\Gamma = 2\pi s$.

The next subsection derives the stationary vortex profile, which provides the

background state for the impurity–vortex models developed later.

2.6.2 Stationary Vortex Solution

To analyse the internal structure of a quantized vortex, we consider stationary solutions of the Gross–Pitaevskii equation (GPE) in two spatial dimensions. In the dimensionless units introduced above, the time-independent GPE for a homogeneous system without external potential is

$$\psi = -\nabla^2 \psi + |\psi|^2 \psi. \quad (2.6.2)$$

For an axisymmetric vortex we write the condensate wavefunction in polar coordinates (r, ϕ) as

$$\psi(r, \phi) = f(r)e^{is\phi},$$

where $f(r)$ is a real radial amplitude. Substituting this form into Eq. (2.6.2) and expressing the Laplacian in polar coordinates gives

$$f'' + \frac{1}{r}f' - \frac{s^2}{r^2}f + f - f^3 = 0, \quad (2.6.3)$$

where primes denote derivatives with respect to r . This nonlinear ordinary differential equation describes the balance between radial kinetic energy, angular momentum, and the interaction energy within the vortex core.

The boundary conditions are set by physical requirements:

$$f(r \rightarrow 0) \sim r^{|s|}, \quad f(r \rightarrow \infty) \rightarrow \sqrt{\rho_0}, \quad (2.6.4)$$

where $\rho_0 = 1$ is the bulk condensate density. The near-origin behaviour $f(r) \sim r^{|s|}$ ensures that the centrifugal term $s^2 f/r^2$ remains finite, keeping the wavefunction regular at $r = 0$. At large distances, the linear and nonlinear term balance ($f = f^3$), giving $f \rightarrow \sqrt{\rho_0} \simeq 1$. The vortex core, where $f(r) \ll \sqrt{\rho_0}$, has

a characteristic size on the order of the healing length ξ (which is unity in the chosen length units) [6].

This radially symmetric solution represents the structure of a single quantized vortex and forms the basis for approximate analytical descriptions and for initial conditions in dynamical simulations [46, 47, 19].

2.6.3 The Padé Approximation for the Vortex Profile

The vortex profile can be computed numerically from Eq. (2.6.3), but closed-form approximations are useful for analytical work and as initial conditions in simulations. A commonly used method is the Padé approximation, which models the dimensionless density $\rho(r) = f^2(r)$ as a rational function. For a vortex of winding number s , the density profile is approximated by

$$\rho_s(\tilde{r}) = \frac{\tilde{r}^{2|s|}(a_1 + a_2\tilde{r}^2)}{1 + b_1\tilde{r}^2 + b_2\tilde{r}^4}. \quad (2.6.5)$$

Only even powers of $\tilde{r}$ appear because $\rho(r) = |f(r)|^2$ is an even function of r (radial symmetry), so its Taylor series about $r = 0$ contains no odd terms. The exponents and degrees in (2.6.5) are chosen so that the known small r behaviour $\rho(r) \sim r^{2|s|}$ is enforced by the factor $\tilde{r}^{2|s|}$, and the far field approaches the bulk value $\rho(r) \rightarrow 1$ as $\tilde{r} \rightarrow \infty$. In practice, the Padé form is constructed by matching the series expansion of the exact Gross–Pitaevskii vortex solution at small and large $\tilde{r}$ up to fourth order.

Singly quantized vortex ($|s| = 1$). Matching (2.6.5) to the numerical solution of Eq. (2.6.3) and enforcing the near-core and far-field expansions yields the coefficients obtained by Berloff [4] :

$$a_1 = \frac{11}{32}, \quad b_1 = \frac{5 - 32a_1}{48 - 192a_1}, \quad a_2 = a_1 \left(b_1 - \frac{1}{4} \right), \quad b_2 = a_2. \quad (2.6.6)$$

These values are obtained by matching the Padé series to the numerical profile so that the small- $\tilde{r}$ and large- $\tilde{r}$ asymptotics (up to order $\tilde{r}^4$ and $\tilde{r}^{-4}$, respectively) coincide. The resulting rational form reproduces the near-core behaviour $\rho(\tilde{r}) \sim \tilde{r}^2$ and smoothly approaches the bulk density $\rho_0 = 1$ as $\tilde{r} \rightarrow \infty$.

Doubly quantized vortex ($|s| = 2$). For a doubly quantized vortex, Berloff [4] derived a Padé approximation valid for integer winding numbers. For $|s| = 2$ in a uniform condensate, the (dimensionless) density profile can be written as

$$\rho_{|s|=2}(\tilde{r}) = \frac{\tilde{r}^4(a_1 + a_2\tilde{r}^2)}{1 + b_1\tilde{r}^2 + b_2\tilde{r}^4 + b_3\tilde{r}^6}, \quad (2.6.7)$$

with coefficients obtained by matching the small- and large- $\tilde{r}$ asymptotics of the Gross–Pitaevskii solution:

$$a_1 = 0.0256, \quad a_2 = 0.0006264, \quad b_1 = 0.1911, \quad b_2 = 0.01970, \quad b_3 = 0.0006264.$$

This form enforces the correct near-core scaling $f \sim \tilde{r}^2$ (hence $\rho \sim \tilde{r}^4$) and recovers $\rho \rightarrow 1$ as $\tilde{r} \rightarrow \infty$. The higher-order denominator terms encode the slower rise of the $|s| = 2$ profile toward the bulk value compared with the singly quantized case (see Fig. 2.6.2).

These Padé approximations are used as initial conditions in the simulations presented in Chapter 6.

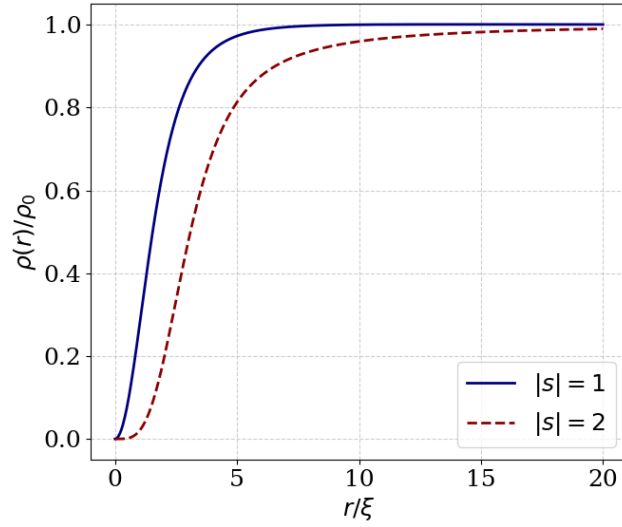


Figure 2.6.2: Padé approximations of the stationary vortex density profiles for singly ($|s| = 1$) and doubly ($|s| = 2$) quantized vortices. The $|s| = 2$ vortex shows a broader core and slower recovery to the bulk density.

2.6.4 Summary

In this chapter, we developed the theoretical tools needed to describe the Bose–Einstein condensate within the Gross–Pitaevskii framework. We first introduced the Gross–Pitaevskii equation and its mean-field derivation, then obtained a dimensionless formulation and the quasi-two-dimensional limit appropriate to strongly confined geometries. We discussed the main conserved quantities and the hydrodynamic (Madelung) form of the equation, which clarifies the interpretation of the condensate as an inviscid quantum fluid. Finally, we analysed the structure of quantized vortices, derived the stationary vortex profile, and introduced Padé approximations for singly and doubly quantized vortices. These results provide the background against which impurity–vortex interactions and coupled dynamics will be investigated in subsequent chapters.

3

The Schrödinger Equation

We consider a single quantum impurity embedded in an external environment, such as a Bose–Einstein condensate (BEC). The impurity is modeled as a distinguishable, non-relativistic particle of mass m_i , evolving under the influence of an external trapping potential $V(\mathbf{r})$. Throughout this chapter the environment is treated as static: feedback of the impurity on the background medium is neglected and will be addressed in later chapters. This chapter establishes the general framework for analyzing impurity localization using the Schrödinger equation, before exploring specific potential types in later chapters.

3.1 Model Setup

We begin with the general three-dimensional Schrödinger equation for a single impurity and subsequently specialise to effective one- and two-dimensional descriptions where appropriate. The impurity wavefunction $\phi_{3D}(\mathbf{r}, t)$ satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \phi_{3D}(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m_i} \nabla^2 + V(\mathbf{r}) \right] \phi_{3D}(\mathbf{r}, t), \quad (3.1.1)$$

where ∇^2 denotes the Laplacian in the relevant spatial dimension and $V(\mathbf{r})$ is the external potential.

For stationary states, we apply the ansatz:

$$\phi_{3D}(\mathbf{r}, t) = \phi_{3D}(\mathbf{r}) e^{-iEt/\hbar}$$

which leads to the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m_i} \nabla^2 \phi_{3D}(\mathbf{r}) + V(\mathbf{r}) \phi_{3D}(\mathbf{r}) = E \phi_{3D}(\mathbf{r}). \quad (3.1.2)$$

This equation determines the spatial structure of stationary impurity states. Discrete eigenvalues E correspond to quantised bound-state energies, while continuum eigenvalues describe extended or scattering states. In the following sections, we examine representative choices of $V(\mathbf{r})$, including finite square wells, harmonic traps, and vortex-induced effective potentials.

Two-Dimensional Formulation

As described in chapter 2, in many ultracold atom experiments, the system is effectively two-dimensional due to tight harmonic confinement along one spatial direction (typically the z -axis). This strong confinement restricts motion along z , so the impurity dynamics can be assumed to occur entirely in the xy -plane.

After integrating out the tightly confined z -direction, the effective two-dimensional impurity wavefunction $\phi_{2D}(\mathbf{r})$ is governed by the two-dimensional, time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m_i} \nabla_{2D}^2 \phi_{2D} + V_{2D}(x, y) \phi_{2D} = E \phi_{2D}, \quad (3.1.3)$$

where $\nabla_{2D}^2 = \partial_x^2 + \partial_y^2$, and $V_{2D}(x, y)$ denotes the effective two-dimensional potential resulting from the dimensional reduction.

Radial Symmetry and Angular Decomposition

When the trapping potential is radially symmetric, it is convenient to transform to polar coordinates (r, θ) . In this coordinate system, the two-dimensional Laplacian takes the form:

$$\nabla_{2D}^2 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}. \quad (3.1.4)$$

We then seek separable solutions of the form:

$$\phi_{2D}(r, \theta) = g(r)e^{i\ell\theta}, \quad \ell \in \mathbb{Z},$$

where ℓ is the azimuthal angular-momentum quantum number and labels states with phase winding $e^{i\ell\theta}$ around the origin. Substituting this ansatz into Eq. (3.1.3), yields the radial Schrödinger equation:

$$-\frac{\hbar^2}{2m_i} \left[\frac{d^2 g}{dr^2} + \frac{1}{r} \frac{dg}{dr} - \frac{\ell^2}{r^2} g \right] + V(r)g(r) = Eg(r). \quad (3.1.5)$$

The term $\ell^2/(2m_i r^2)$ acts as a centrifugal barrier, suppressing localisation near the origin for $|\ell| > 0$.

This radial formulation is particularly well suited to modelling impurity behaviour in circular wells, harmonic traps and vortex cores, all of which possess radial symmetry. In the following sections, we consider each of these choices of $V(r)$ in turn and show how they give rise to distinct bound-state spectra and localisation properties for the impurity.

3.2 1D Finite Potential Well

We consider the motion of a quantum particle confined in a one-dimensional finite square well. This well is parity-symmetric and provides exact analytical expressions for the bound state wavefunctions and energy levels. It is included

here as a simple, instructive example for the more complex two-dimensional cases discussed later.

The potential is defined as

$$V(x) = \begin{cases} V_0, & \text{for } |x| > L, \\ 0, & \text{for } |x| \leq L, \end{cases} \quad V_0 > 0, \quad (3.2.1)$$

representing a finite well of width $2L$ with walls of height V_0 . The potential profile and regions are shown schematically in Figure 3.2.1.

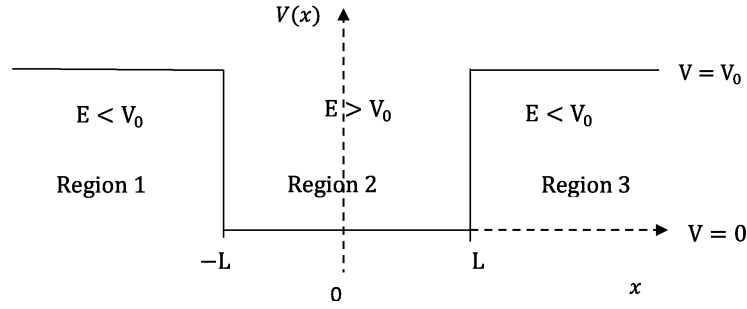


Figure 3.2.1: Schematic of a one-dimensional finite square well of width $2L$ and wall height V_0 .

The stationary states satisfy the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m_i} \frac{d^2}{dx^2} + V(x) \right) \phi(x) = E\phi(x) \quad (3.2.2)$$

where m_i is the impurity mass. For bound states we have $0 < E < V_0$.

Region 1: $x \leq -L$, $V(x) = V_0$. In this region Eq. (3.2.2) reduces to

$$\frac{d^2\phi}{dx^2} = \alpha^2\phi, \quad \text{where} \quad \alpha^2 = \frac{2m_i}{\hbar^2}(V_0 - E) \quad (3.2.3)$$

with $\alpha > 0$ for $E < V_0$. The general solution is

$$\phi_1(x) = F e^{\alpha x} + Q e^{-\alpha x},$$

Normalisability requires $\phi(x) \rightarrow 0$ as $x \rightarrow -\infty$, which implies that the exponentially growing term must vanish, hence $Q = 0$, so

$$\phi_1(x) = F e^{\alpha x}$$

Region 2: $-L < x < L$, $V(x) = 0$.

Here Eq. (3.2.2) becomes

$$\left(-\frac{\hbar^2}{2m_i}\right) \frac{d^2\phi}{dx^2} = E\phi(x) \quad \Rightarrow \quad \frac{d^2\phi}{dx^2} = -\frac{2m_i E}{\hbar^2} \phi(x)$$

Defining

$$K^2 = \frac{2m_i E}{\hbar^2},$$

we have

$$\frac{d^2\phi}{dx^2} = -K^2 \phi(x),$$

with general solution

$$\phi_2(x) = A \sin(Kx) + B \cos(Kx)$$

By parity symmetry, the bound states can be chosen to be either even or odd:

$$\phi_2(x) = \begin{cases} A \cos(Kx) & \text{even states} \\ A \sin(Kx) & \text{odd states} \end{cases}$$

Region 3: $x \geq L$, $V(x) = V_0$

The equation has the same form as Region 1:

$$\frac{d^2\phi}{dx^2} = \alpha^2\phi(x), \quad \text{where} \quad \alpha^2 = \frac{2m_i}{\hbar^2}(V_0 - E)$$

Since $E < V_0$, we have $\alpha^2 > 0$ and real.

The general solution is:

$$\phi_3(x) = Ce^{-\alpha x} + De^{\alpha x}$$

Normalisability as $x \rightarrow \infty$ requires $D = 0$, so

$$\phi_3(x) = Ce^{-\alpha x}$$

Continuity of ϕ and $d\phi/dx$ at $x = \pm L$ yields the transcendental conditions

$$K \tan(KL) = \alpha \quad (\text{even states}), \quad K \cot(KL) = -\alpha \quad (\text{odd states}).$$

Solving these relations graphically or numerically gives the allowed bound-state energies $E < V_0$.

Numerical Solution of the 1D Finite Square Well

To obtain the bound state energies and wavefunctions of the one-dimensional finite square well, we solve the time-independent Schrödinger equation numerically using a finite difference method. We seek bound-state solutions satisfying $E < V_0$ and $\phi(x) \rightarrow 0$ as $|x| \rightarrow \infty$.

The infinite domain is truncated to a finite box $x \in [-X, X]$ with X chosen to be several times larger than the half-width L . Homogeneous Dirichlet boundary conditions $\phi(\pm X) = 0$ are imposed, which approximate the exponential decay of the bound states outside the well. The domain is discretised using a uniform grid of N points with spacing $\Delta x = 2X/(N - 1)$. The second derivative is approximated at interior grid points by the standard three-point finite-difference

stencil

$$\frac{d^2\phi}{dx^2} \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

This leads to a tridiagonal kinetic-energy matrix $\mathbf{T}$ of the form

$$\mathbf{T} = -\frac{\hbar^2}{2m_i} \cdot \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \dots \\ 1 & -2 & 1 & \dots \\ 0 & 1 & -2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad (3.2.4)$$

while the potential-energy operator is represented by the diagonal matrix $\mathbf{V}$ constructed from the grid values of $V(x)$. The total Hamiltonian is

$$\mathbf{H} = \mathbf{T} + \mathbf{V}$$

We solve the matrix eigenvalue problem:

$$\mathbf{H}\phi_n = E_n\phi_n,$$

using the `eigsh` routine (SciPy, Python), which calls the ARPACK (ARnoldi PACKage) library. ARPACK employs an iterative Arnoldi–Lanczos algorithm to extract a small number of eigenvalues and eigenvectors of large, sparse Hermitian matrices efficiently, without full diagonalisation.

Each wavefunction is normalised such that

$$\int_{-X}^X |\phi_n(x)|^2 dx = 1.$$

The potential and normalised wavefunctions are plotted together. To emphasise the energy levels, we plot the probability densities $|\phi_n(x)|^2$, each offset vertically by its corresponding eigenenergy E_n , as shown in Fig. 3.2.2. This provides an intuitive picture of the bound states and how they are confined within the well.

The number of bound states is finite and increases with both V_0 and L . Each

bound state corresponds to a spatially localised wavefunction with n internal nodes (excluding the boundaries). The ground state is nodeless, while higher excited states have increasing energy and additional nodes.

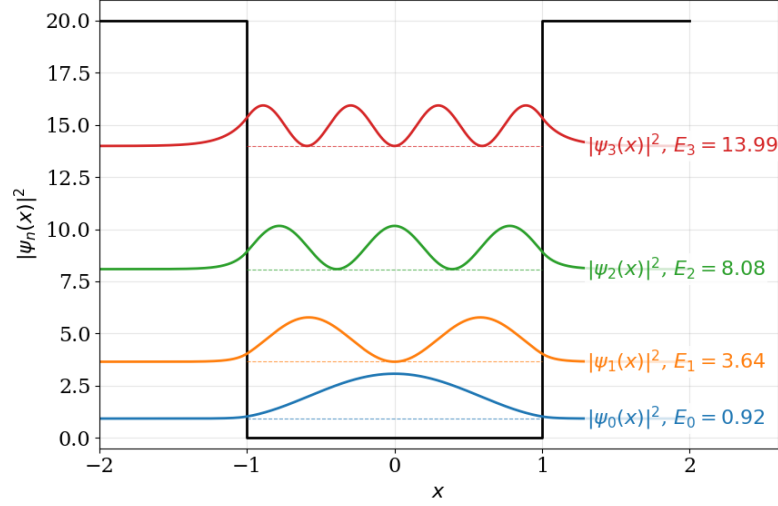


Figure 3.2.2: Bound-state probability densities $|\phi_n(x)|^2$ and corresponding eigenenergies E_n for a finite square potential well with half-width L and wall height V_0 . The potential $V(x)$ is shown as a closed box. Each density curve is vertically offset by its eigenenergy, and labels outside the well indicate the state index and energy value (starting from E_0 for the ground state). All quantities are expressed in dimensionless units.

Convergence was verified by varying both the grid resolution N and the domain size. Increasing N from 500 to 1500 points and extending the spatial range from $[-2L, 2L]$ to $[-3L, 3L]$ changed the lowest eigenenergies by less than 10^{-4} . This confirms that the discretisation and domain truncation do not affect the reported bound-state energies within the stated numerical accuracy.

For energies above the potential height ($E > V_0$), the particle is no longer confined within the well. The corresponding eigenfunctions are oscillatory across the whole domain and represent delocalised or scattering states.

This simple model captures essential quantum features such as confinement (localisation within the well), tunnelling (exponential penetration of the wavefunction into the barrier), and the discrete nature of the bound-state spectrum. These features reappear in higher-dimensional and more realistic

impurity-trapping geometries considered later in this thesis.

3.3 2D Finite Potential Well

We extend the analysis to a two-dimensional system with circular symmetry, relevant to quasi-2D condensates where tight harmonic confinement along z freezes motion in that direction (see the discussion in Sec. 3.1). The impurity dynamics are then effectively confined to the xy -plane.

The potential is defined in the same piecewise style as the 1D case:

$$V(r) = \begin{cases} 0 & \text{for } r \leq R, \\ V_0 & \text{for } r > R, \end{cases} \quad V_0 > 0 \quad (3.3.1)$$

where R is the radius of the well and V_0 its height. Bound states satisfy $0 < E < V_0$.

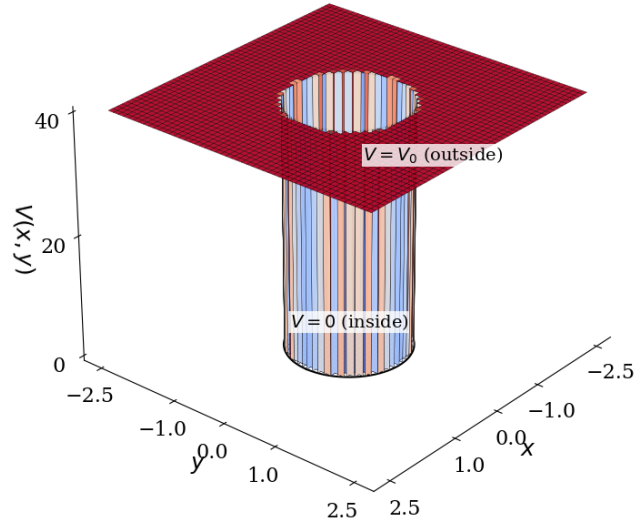


Figure 3.3.1: A 3D visualization of a 2D finite circular potential well of radius R and wall height V_0 .

We now solve the radial Schrödinger equation (3.1.5) in two regions inside and outside the well. As in other problems with circular symmetry, the solutions are expressed in terms of Bessel and modified Bessel functions.

Inside the well ($r \leq R$, $V = 0$). With $V = 0$, Eq. (3.1.5) becomes

$$\frac{d^2 g_\ell}{dr^2} + \frac{1}{r} \frac{dg_\ell}{dr} + \left(k^2 - \frac{\ell^2}{r^2}\right) g_\ell(r) = 0, \quad k = \frac{\sqrt{2m_i E}}{\hbar}.$$

The general solution is a linear combination of Bessel functions of order ℓ :

$$g_\ell^{(\text{in})}(r) = A J_\ell(kr) + C Y_\ell(kr).$$

The first kind, $J_\ell(kr)$, is finite at $r = 0$ and represents the physical solution inside the well, whereas the second kind, $Y_\ell(kr)$, diverges at the origin and must be excluded.

Regularity ($|g_\ell(r)| < \infty$ as $r \rightarrow 0$) therefore requires $C = 0$, so

$$g_\ell^{(\text{in})}(r) = A J_\ell(kr), \quad J_\ell(kr) \sim \frac{(kr)^\ell}{2^\ell \ell!} \quad \text{as } r \rightarrow 0.$$

The node structure of the bound states is set by the zeros of J_ℓ : deeper or larger wells (larger kR) admit more zeros and hence more bound states for a given ℓ .

Outside the well ($r > R$, $V = V_0$, $E < V_0$). For $r > R$ the radial Schrödinger equation becomes

$$\frac{d^2 g_\ell}{dr^2} + \frac{1}{r} \frac{dg_\ell}{dr} - \left(\lambda^2 + \frac{\ell^2}{r^2}\right) g_\ell(r) = 0, \quad \lambda = \frac{\sqrt{2m_i (V_0 - E)}}{\hbar}.$$

The general solution is a linear combination of modified Bessel functions of order ℓ ,

$$g_\ell^{(\text{out})}(r) = B K_\ell(\lambda r) + D I_\ell(\lambda r).$$

These functions describe exponential behaviour rather than oscillations. The modified Bessel function of the second kind, $K_\ell(\lambda r)$, decays as $e^{-\lambda r}/\sqrt{r}$ for large r and therefore represents the physically acceptable bound-state tail, whereas $I_\ell(\lambda r)$ grows exponentially and must be discarded to ensure normalisability. We therefore set $D = 0$ and retain

$$g_\ell^{(\text{out})}(r) = B K_\ell(\lambda r).$$

Matching conditions and bound-state quantisation. Normalisability requires decay as $r \rightarrow \infty$, which is ensured by the choice of K_ℓ outside. Continuity of g_ℓ and dg_ℓ/dr at $r = R$ gives

$$A J_\ell(kR) = B K_\ell(\lambda R), \quad A k J'_\ell(kR) = B \lambda K'_\ell(\lambda R). \quad (3.3.2)$$

Eliminating the ratio A/B yields the transcendental equation for the allowed bound-state energies $0 < E < V_0$:

$$k \frac{J'_\ell(kR)}{J_\ell(kR)} = \lambda \frac{K'_\ell(\lambda R)}{K_\ell(\lambda R)}. \quad (3.3.3)$$

For each angular-momentum quantum number ℓ , Eq. (3.3.3) is solved numerically to obtain the discrete bound-state energies. The number of bound states increases with V_0 and R , and decreases with $|\ell|$ due to the centrifugal term ℓ^2/r^2 which pushes probability density away from the origin.

Numerical solution. The bound-state energies are obtained by solving Eq. (3.3.3) for each angular-momentum quantum number ℓ using a one-dimensional root-finding method, such as Brent's algorithm. For a given ℓ , we define the matching function

$$f_\ell(E) = k \frac{J'_\ell(kR)}{J_\ell(kR)} - \lambda \frac{K'_\ell(\lambda R)}{K_\ell(\lambda R)},$$

where

$$k = \frac{\sqrt{2m_i E}}{\hbar}, \quad \lambda = \frac{\sqrt{2m_i (V_0 - E)}}{\hbar}.$$

The bound-state energies correspond to the zeros of $f_\ell(E)$ in the interval $0 < E < V_0$. These zeros are located numerically by scanning over energy and applying the root-finder on intervals where $f_\ell(E)$ changes sign. Once a bound-state energy E is found, the corresponding radial wavefunction is constructed piecewise from J_ℓ inside the well and K_ℓ outside, with the amplitudes fixed by continuity of g_ℓ and dg_ℓ/dr at $r = R$. The resulting eigenfunctions are oscillatory inside the well and exponentially decaying outside, as illustrated in Fig. 3.3.2.

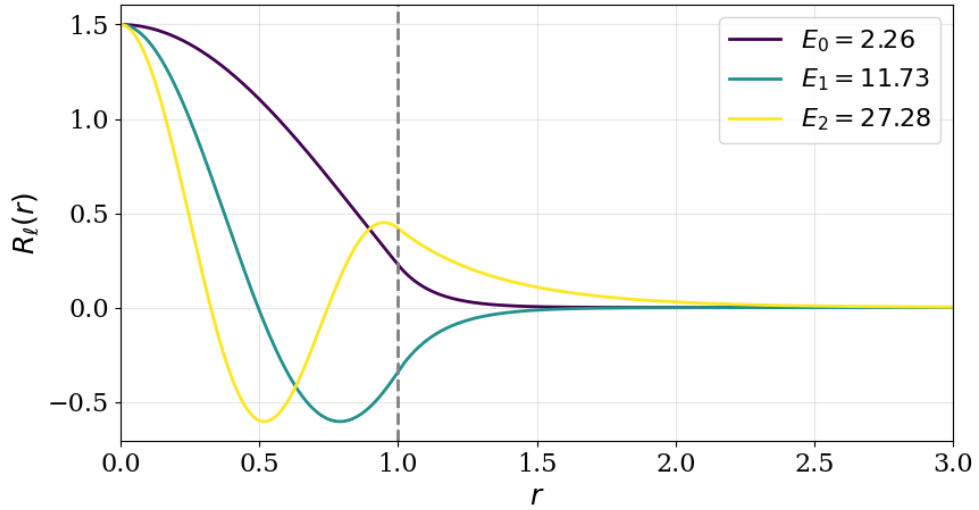


Figure 3.3.2: Radial wavefunctions $g_\ell(r)$ for the three lowest bound states in a 2D finite circular well. The curves are oscillatory for $r \leq 1$ and decay for $r > 1$; the dashed line marks $r = 1$.

3.4 The Harmonic Oscillator Potential

The harmonic oscillator is analytically solvable and has an evenly spaced spectrum. It provides a good approximation near equilibrium and is widely used to model particle confinement in Bose-Einstein condensates [24, 46]. The trapping potential is

$$V(x) = \frac{1}{2}m_i\omega^2x^2, \quad (3.4.1)$$

where m_i is the particle mass and ω is the trap frequency. The corresponding time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m_i} \frac{d^2\phi(x)}{dx^2} + \frac{1}{2}m_i\omega^2 x^2 \phi(x) = E\phi(x). \quad (3.4.2)$$

To obtain normalisable solutions of (3.4.2), the wavefunction must vanish as $|x| \rightarrow \infty$. Because the potential grows quadratically, $\phi(x)$ is expected to have an exponential (Gaussian) decay at large $|x|$. We therefore separate this known asymptotic behaviour by writing the wavefunction as a Gaussian factor multiplied by a polynomial function:

$$\phi(x) = e^{-\alpha x^2/2} h(x), \quad \alpha = \frac{m_i\omega}{\hbar}.$$

Here $h(x)$ represents the polynomial part of the wavefunction, while the Gaussian factor ensures the correct decay for large $|x|$. Differentiating gives

$$\phi' = e^{-\alpha x^2/2} (h' - \alpha x h), \quad \phi'' = e^{-\alpha x^2/2} (h'' - 2\alpha x h' + (\alpha^2 x^2 - \alpha) h).$$

Substituting into (3.4.2) cancels the x^2 -terms and yields

$$h'' - 2\alpha x h' + \alpha \left(\frac{2E}{\hbar\omega} - 1 \right) h = 0. \quad (3.4.3)$$

We expand $h(x)$ as a power series, $h(x) = \sum_{j=0}^{\infty} a_j x^j$. Inserting this into (3.4.3) gives the recurrence relation

$$a_{j+2} = \frac{\alpha (2j+1 - \frac{2E}{\hbar\omega})}{(j+2)(j+1)} a_j, \quad j = 0, 1, 2, \dots \quad (3.4.4)$$

valid for all j .

To keep the wavefunction normalisable, the series for $h(x)$ must end after a finite number of terms; otherwise, $\phi(x)$ would diverge at large $|x|$. This happens only

when the numerator in (3.4.4) vanishes for some $j = n$, giving

$$2j + 1 - \frac{2E}{\hbar\omega} = 0.$$

Setting $j = n$ yields the quantised energies

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots \quad (3.4.5)$$

so the series stops at order n , and $h(x)$ becomes a polynomial of degree n (a Hermite polynomial). The corresponding normalised eigenfunctions are

$$\phi_n(x) = \left(\frac{m_i\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m_i\omega}{\hbar}}x\right) e^{-\frac{m_i\omega x^2}{2\hbar}}. \quad (3.4.6)$$

with Hermite polynomials H_n . These eigenfunctions alternate in parity: even n correspond to even functions, and odd n to odd functions. Each function ϕ_n has n nodes, and the classical turning points, defined as the positions where $E_n = V(x)$ and the classical particle would have zero kinetic energy, are located at:

$$x = \pm \sqrt{\frac{2E_n}{m_i\omega^2}}.$$

To verify the analytical solutions, Eq. (3.4.2) was solved numerically using the finite-difference method. The spatial domain was discretised into a uniform grid, and the second derivative was approximated by a three-point finite-difference stencil, leading to a sparse matrix representation of the Hamiltonian. The lowest eigenvalues and eigenfunctions were then obtained using the `eigsh` routine from the SciPy library, which efficiently diagonalises real symmetric sparse matrices. The numerical results reproduce the analytical predictions (3.4.5)-(3.4.6), showing identical energy spacing and wavefunction symmetry. Figure 3.4.1 compares the analytical Hermite-Gaussian forms with the numerical solutions, demonstrating excellent agreement for the lowest states considered.

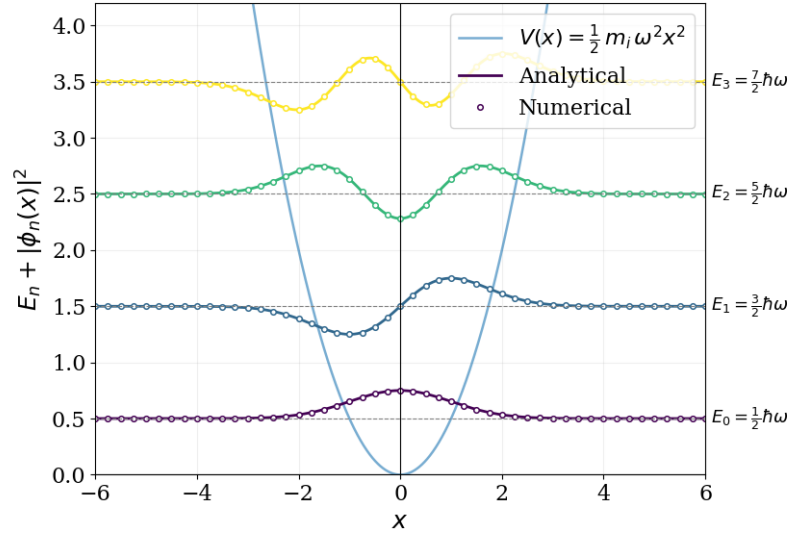


Figure 3.4.1: Comparison of analytical (solid) and numerical (markers) solutions of the quantum harmonic oscillator. The potential $V(x) = \frac{1}{2}m_i\omega^2x^2$ is shown in blue. Each wavefunction $|\phi_n(x)|^2$ is offset by its energy level $E_n = \hbar\omega(n + \frac{1}{2})$. Numerical results agree closely with the analytical Hermite-Gaussian forms.

The harmonic oscillator provides a good approximation for the local dynamics of impurities or particles trapped in weakly perturbed condensate backgrounds, where the potential near equilibrium is approximately quadratic. Similarly, optical and magnetic traps used to confine ultracold atoms are often well described by harmonic potentials around their minima. For these reasons, the harmonic oscillator serves as a theoretical benchmark for more complex trapping configurations, such as impurity localisation within vortex cores [24, 56, 59, 46].

3.5 Impurity Trapped in a Vortex Core

As shown in Sec. 2.6.1, the superfluid density in a Bose-Einstein condensate (BEC) vanishes at the vortex core and approaches a constant value far away. This density depletion creates an effective trapping potential for a quantum impurity immersed in the condensate. For a repulsive impurity-boson interaction, the impurity experiences a potential minimum at the vortex centre and becomes

energetically localised there [46, 5, 15].

1. Vortex Background and Effective Potential

The condensate wavefunction around a singly quantized vortex in 2D can be written as:

$$\psi(r, \theta) = f(r) e^{i\theta}, \quad (3.5.1)$$

where $f(r)$ vanishes at the core $r = 0$ and approaches the bulk amplitude $\sqrt{\rho_0}$ as $r \rightarrow \infty$. The corresponding condensate density is $\rho(r) = |f(r)|^2$. We model the vortex density using the Padé profile for a singly quantised vortex Eq. (2.6.5) with coefficients given in [4]. For a repulsive contact interaction of strength $\chi > 0$, the impurity experiences the effective potential

$$V_{\text{eff}}(r) = \chi \rho(r). \quad (3.5.2)$$

At the vortex core $\rho(0) \approx 0$, while far from the core $\rho(r) \rightarrow \rho_0$, so $V_{\text{eff}}(r)$ has a minimum at the vortex centre and tends to $\chi \rho_0$ at large r . This forms a finite-depth potential well localised around $r = 0$, which can trap one or more bound impurity states.

It is convenient to introduce the dimensionless radius $\tilde{r} = r/\xi$, where ξ is the healing length, and the dimensionless vortex density $\rho_{|s|=1}(\tilde{r}) = \rho(r)/\rho_0$, with $\rho_{|s|=1}(0) = 0$ and $\rho_{|s|=1}(\tilde{r} \rightarrow \infty) = 1$. In these units the effective potential becomes

$$V_{\text{eff}}(\tilde{r}) = \chi \rho_{|s|=1}(\tilde{r}). \quad (3.5.3)$$

In this chapter we neglect the back-action of the impurity on the condensate, the vortex density is treated as fixed. This approximation is valid when the impurity concentration is low and χ is not so large that it significantly distorts the condensate profile; a self-consistent treatment including back-action will be developed in later chapters.

Focusing on radially symmetric states ($\ell = 0$), the impurity wavefunction $\phi(r)$ satisfies the radial Schrödinger equation

$$-\frac{\hbar^2}{2m_i} \left(\frac{d^2\phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} \right) + V_{\text{eff}}(r) \phi(r) = E \phi(r), \quad (3.5.4)$$

with $V_{\text{eff}}(r) = \chi \rho(r)$ as defined above. This equation is analogous to that of a 2D finite circular well, but with a smooth, physically motivated potential arising from the BEC density. The shape and depth of the well are determined by χ , the healing length ξ and the bulk density ρ_0 .

Depending on the strength χ and the healing length ξ , the potential well may support one or more bound states. These correspond to impurity states localised within the vortex core, analogous to bound states in a 2D finite potential well.

To obtain the bound-state energies and wavefunctions, we numerically solved Eq. (3.5.4) using a finite-difference discretization of the radial domain. The effective potential $V_{\text{eff}}(r)$ is computed from the Padé vortex density profile. Dirichlet boundary conditions $\phi(r_{\text{max}}) = 0$ are imposed to approximate the decay of bound states. The resulting matrix eigenvalue problem is solved to extract the lowest few eigenvalues and eigenfunctions. Convergence is checked by refining the radial grid and increasing r_{max} .

The numerical results confirm that the impurity localizes near the vortex centre and that the number of supported bound states increases with the coupling strength χ and bulk density ρ_0 . The ground state is sharply localised around $r = 0$, while excited bound states may extend to larger radii and can approach the continuum and become weakly bound (or quasi-bound) if the well is shallow.

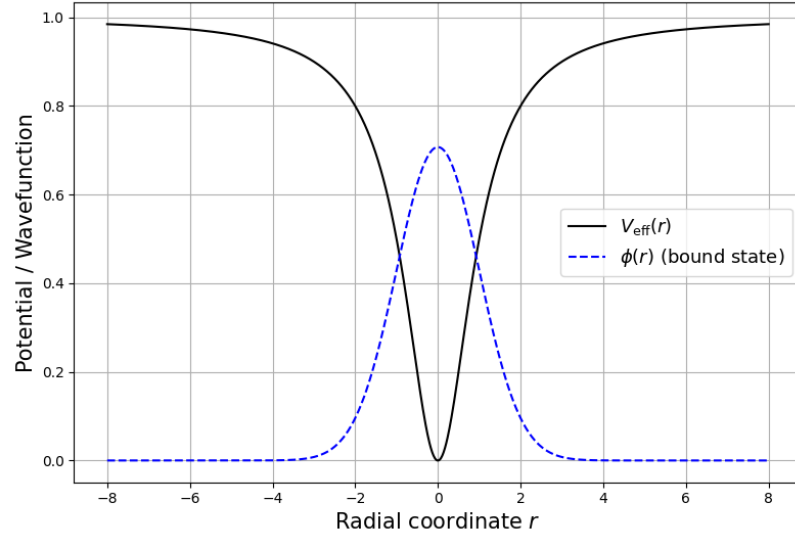


Figure 3.5.1: Effective potential $V_{\text{eff}}(r) = \chi \rho(r)$ for an impurity in the presence of a BEC vortex. The density dip at the vortex core produces a local minimum of the effective potential, forming a finite well that can support impurity bound states. The lowest bound-state wavefunction is localised near the potential minimum.

Vortex-core localisation thus provides a realistic and experimentally relevant mechanism for controlling impurity states in condensates [68, 11].

3.6 Summary

In this chapter we developed the theoretical framework for describing impurity localisation in externally imposed potentials. By analysing the Schrödinger equation in one- and two-dimensional finite wells and in the harmonic oscillator, we obtained analytically solvable benchmarks that clarify how the depth, width and curvature of a trapping potential determine the existence and structure of bound states.

We then applied the same framework to the physically motivated case of impurity trapping in a vortex core, where the condensate density depletion creates an effective finite well. Solving the corresponding radial Schrödinger equation showed how the number and shape of vortex-core bound states depend on the impurity–boson interaction strength, the healing length, and the bulk

density.

The results of this chapter provide the static foundation for the dynamical impurity–vortex studies that follow. In the next chapter we introduce the Gross–Clark model, which incorporates two-way coupling between the impurity and the condensate, enabling us to investigate how the impurity influences vortex motion, generates deformations, and interacts with other excitations in the superfluid.

The Gross-Clark Model

The presence of impurities in superfluid systems modifies the properties of quantised vortices and can influence dissipation, coherence, and structure formation [21]. This chapter studies BEC–impurity interactions within the Gross–Clark (GC) framework.

We consider a Bose–Einstein condensate (BEC) and a single impurity. Such systems arise in ultracold atom experiments, where impurities may be realised through additional atomic species, tightly focused optical potentials, or engineered trapping configurations. In this context, impurities can interact strongly with the condensate background, leading to effects such as vortex pinning, local density depletion, and modifications of the vortex core profile [21].

The analysis proceeds in two steps. First, we introduce the Gross–Clark model and reduce it to a quasi-two-dimensional form appropriate for a strongly confined geometry. Second, we derive its dimensionless formulation and identify the key parameters controlling BEC–impurity interactions. This sets the theoretical and numerical framework for the study of BEC–impurity systems.

4.1 Model Setup and Physical Assumptions

As discussed in chapter 2, the Gross–Pitaevskii (GP) equation describes the order parameter of a BEC in the zero-temperature limit [53, 9]. Introducing an impurity

into the condensate, such as one atom of a different species, couples it to the surrounding bosons and modifies both the impurity dynamics and the condensate. This coupling can be captured, in a mean-field description, by a GP equation combined with a Schrödinger equation for the impurity, where the boson-impurity interaction depends on the local densities of each wave function. Let $\psi(x, y, z, t)$ be the BEC wave function and $\phi(x, y, z, t)$ be the impurity wave function. The Gross-Clark (GC) model [66] in three dimensions is

$$i\hbar \frac{\partial \psi_{3D}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_{3D} + (g|\psi_{3D}|^2 + \chi|\phi_{3D}|^2)\psi_{3D}, \quad (4.1.1a)$$

$$i\hbar \frac{\partial \phi_{3D}}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla^2 \phi_{3D} + \chi|\psi_{3D}|^2 \phi_{3D}, \quad (4.1.1b)$$

where $\hbar$ is the reduced Planck constant, m is the mass of the bosons that form the BEC, m_i is the impurity mass, g is the boson-boson coupling constant, and χ is the boson-impurity coupling constant.

Note that the right-hand sides of equations (4.1.1) originate from the functional derivatives, namely

$$i\hbar \frac{\partial \psi_{3D}}{\partial t} = \frac{\delta H}{\delta \psi_{3D}^*} \quad \text{and} \quad i\hbar \frac{\partial \phi_{3D}}{\partial t} = \frac{\delta H}{\delta \phi_{3D}^*} \quad (4.1.2)$$

of the Hamiltonian

$$H = \int dV \left[\frac{\hbar^2}{2m} |\nabla \psi_{3D}|^2 + \frac{g}{2} |\psi_{3D}|^4 + \frac{\hbar^2}{2m_i} |\nabla \phi_{3D}|^2 + \chi |\psi_{3D}|^2 |\phi_{3D}|^2 + \frac{1}{2} m \omega_z^2 z^2 |\psi_{3D}|^2 + \frac{1}{2} m_i \omega_{z,i}^2 z^2 |\phi_{3D}|^2 \right]. \quad (4.1.3)$$

We include a harmonic trapping potential along the z -direction for both the condensate and the impurity. The Hamiltonian H is conserved during the time evolution, as are

$$N_\psi = \int |\psi_{3D}|^2 dV, \quad (4.1.4a)$$

$$N_\phi = \int |\phi_{3D}|^2 dV = 1, \quad (4.1.4b)$$

which represents the number of bosons and the number of impurities, here normalised to unity since only one impurity is present.

4.2 2-Dimensional Reduction

During this PhD project, we consider the GC model in quasi-2D. We therefore assume strong harmonic confinement along the z -axis for both the bosons and the impurity, effectively reducing the dynamics to two dimensions. Under tight confinement, it is natural to factorise the wave functions into a static Gaussian along z (up to a phase) and a dynamical field in the (x, y) -plane.

Starting from the three-dimensional Gross-Clark equations (4.1.1), we use the factorised ansatz

$$\begin{aligned}\psi(x, y, z, t) &= \psi_{2D}(x, y, t) \psi_{\text{conf}}(z) e^{-i\omega_z t/2}, \\ \phi(x, y, z, t) &= \phi_{2D}(x, y, t) \phi_{\text{conf}}(z) e^{-i\omega_{z,i} t/2},\end{aligned}\tag{4.2.1}$$

where ω_z and $\omega_{z,i}$ represent the trapping frequencies of the harmonic potential(s)¹ acting on the bosons and the impurity, respectively. The longitudinal wave functions are taken as the normalised ground states of the one-dimensional harmonic oscillator,

$$\psi_{\text{conf}}(z) = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega_z z^2}{2\hbar}\right), \quad \phi_{\text{conf}}(z) = \left(\frac{m_i\omega_{z,i}}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m_i\omega_{z,i} z^2}{2\hbar}\right),\tag{4.2.2}$$

satisfying

$$\int_{-\infty}^{\infty} |\psi_{\text{conf}}(z)|^2 dz = 1, \quad \int_{-\infty}^{\infty} |\phi_{\text{conf}}(z)|^2 dz = 1.\tag{4.2.3}$$

The corresponding harmonic-oscillator lengths are

$$a_z = \sqrt{\frac{\hbar}{m\omega_z}}, \quad a_i = \sqrt{\frac{\hbar}{m_i\omega_{z,i}}}.\tag{4.2.4}$$

¹We could imagine the bosons and the impurity trapped by the same harmonic potential that applies the same force, hence resulting in $\omega_z/\omega_{z,i} = \sqrt{m/m_i}$, or two harmonic potentials of different nature, one acting on the bosons and the other on the impurity.

To derive the effective two-dimensional description, we integrate out the z -dependence. We first consider the kinetic term for the condensate. Using $\nabla^2 = \nabla_{2D}^2 + \partial_z^2$ and the factorisation (4.2.1), we obtain

$$\begin{aligned} \frac{\hbar^2}{2m} \int d^3\mathbf{r} |\nabla\psi|^2 &= \frac{\hbar^2}{2m} \int d^2\mathbf{r}_\perp dz \left(|\nabla_{2D}\psi_{2D}|^2 |\psi_{\text{conf}}|^2 + |\psi_{2D}|^2 |\partial_z\psi_{\text{conf}}|^2 \right) \\ &= \frac{\hbar^2}{2m} \int d^2\mathbf{r}_\perp |\nabla_{2D}\psi_{2D}|^2 \\ &\quad + \int d^2\mathbf{r}_\perp |\psi_{2D}|^2 \int dz \left[\frac{\hbar^2}{2m} |\partial_z\psi_{\text{conf}}|^2 + \frac{1}{2} m\omega_z^2 z^2 |\psi_{\text{conf}}|^2 \right]. \end{aligned} \quad (4.2.5)$$

where the second line includes the contribution from the z -kinetic and z -potential energy. Since ψ_{conf} is the ground state of the one-dimensional harmonic oscillator, the z -integral yields the ground-state energy $\hbar\omega_z/2$. An analogous calculation for the impurity yields a contribution $\hbar\omega_{z,i}/2$. We therefore introduce

$$\mu_z = \frac{\hbar\omega_z}{2}, \quad E_z = \frac{\hbar\omega_{z,i}}{2}, \quad (4.2.6)$$

where E_z and μ_z are the effective two-dimensional theory as constant energy shifts associated with the frozen z degree of freedom.

Next, we consider the interaction terms. For the condensate-condensate interaction we find

$$\frac{g}{2} \int d^3\mathbf{r} |\psi|^4 = \frac{g}{2} \int d^2\mathbf{r}_\perp dz |\psi_{2D}|^4 |\psi_{\text{conf}}|^4 = \frac{g_{2D}}{2} \int d^2\mathbf{r}_\perp |\psi_{2D}|^4, \quad (4.2.7)$$

with the effective two-dimensional coupling

$$g_{2D} = g \int_{-\infty}^{\infty} |\psi_{\text{conf}}(z)|^4 dz = \frac{g}{a_z \sqrt{2\pi}}. \quad (4.2.8)$$

Similarly, for the condensate-impurity interaction we obtain

$$\begin{aligned}\chi \int d^3\mathbf{r} |\psi|^2 |\phi|^2 &= \chi \int d^2\mathbf{r}_\perp dz |\psi_{2D}|^2 |\phi_{2D}|^2 |\psi_{\text{conf}}(z)|^2 |\phi_{\text{conf}}(z)|^2 \\ &= \chi_{2D} \int d^2\mathbf{r}_\perp |\psi_{2D}|^2 |\phi_{2D}|^2,\end{aligned}\quad (4.2.9)$$

where

$$\chi_{2D} = \chi \int_{-\infty}^{\infty} |\psi_{\text{conf}}(z)|^2 |\phi_{\text{conf}}(z)|^2 dz = \frac{\chi}{\sqrt{\pi(a_z^2 + a_i^2)}}. \quad (4.2.10)$$

Collecting all contributions, the effective two-dimensional Hamiltonian reads

$$\begin{aligned}\mathcal{H}_{2D} = \int d^2\mathbf{r}_\perp \left[\frac{\hbar^2}{2m} |\nabla_{2D}\psi_{2D}|^2 + \mu_z |\psi_{2D}|^2 + \frac{g_{2D}}{2} |\psi_{2D}|^4 \right. \\ \left. + \frac{\hbar^2}{2m_i} |\nabla_{2D}\phi_{2D}|^2 + E_z |\phi_{2D}|^2 + \chi_{2D} |\psi_{2D}|^2 |\phi_{2D}|^2 \right].\end{aligned}\quad (4.2.11)$$

Functional differentiation of $\mathcal{H}_{2D}$ with respect to ψ_{2D}^* and ϕ_{2D}^* yields the quasi-two-dimensional Gross-Clark equations

$$i\hbar \frac{\partial \psi_{2D}}{\partial t} = -\frac{\hbar^2}{2m} \nabla_{2D}^2 \psi_{2D} + (g_{2D} |\psi_{2D}|^2 + \chi_{2D} |\phi_{2D}|^2) \psi_{2D} - \mu_z \psi_{2D}, \quad (4.2.12a)$$

$$i\hbar \frac{\partial \phi_{2D}}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla_{2D}^2 \phi_{2D} + \chi_{2D} |\psi_{2D}|^2 \phi_{2D} - E_z \phi_{2D}, \quad (4.2.12b)$$

which are the two-dimensional equations used throughout this work [35].

4.3 Dimensionless Form

To reduce the number of parameters and clarify the essential physics of the Gross-Clark model, we nondimensionalise the coupled quasi-two-dimensional equations presented in Eqs. (4.2.12a) and (4.2.12b).

We assume that the BEC has an infinite extension and the impurity's wave function is localised. In the bulk, where the BEC is homogeneous and far away

from the impurity, the solution of Eqs. (4.2.12a) and (4.2.12b) results in

$$\psi_{2D} \xrightarrow{\text{bulk}} \sqrt{\rho_{2D}} e^{-i \frac{\mu_{2D} t}{\hbar}} \quad \text{and} \quad |\phi_{2D}| \xrightarrow{\text{bulk}} 0, \quad \text{with} \quad \mu_{2D} = g_{2D} \rho_{2D} + \mu_z, \quad (4.3.1)$$

where ρ_{2D} is the (surface) density of bosons in the bulk. We therefore define the healing length and the speed of sound in the bulk as

$$\xi = \sqrt{\frac{\hbar^2}{2m\mu_{2D}}}, \quad c = \sqrt{\frac{\mu_{2D}}{m}}. \quad (4.3.2)$$

Spatial variables (x, y) are scaled by the healing length, and the time variable t is rescaled using the healing length and the speed of sound :

$$x' = \frac{x}{\xi}, \quad y' = \frac{y}{\xi}, \quad t' = \frac{t c}{\sqrt{2} \xi}. \quad (4.3.3)$$

The wave-functions ψ_{2D} and ϕ_{2D} are scaled by the square root of the boson surface density and the healing length, respectively, leading to

$$\psi'_{2D} = \frac{\psi_{2D}}{\sqrt{\rho_{2D}}}, \quad \phi'_{2D} = \frac{\phi_{2D}}{\xi}. \quad (4.3.4)$$

Substituting these transformations into eq. (4.2.12) yields the dimensionless quasi-two-dimensional Gross-Clark model [7]

$$i \frac{\partial \psi'_{2D}}{\partial t'} = -\nabla'^2_{2D} \psi'_{2D} + |\psi'_{2D}|^2 \psi'_{2D} + \kappa |\phi'_{2D}|^2 \psi'_{2D} - \psi'_{2D}, \quad (4.3.5a)$$

$$i\tau \frac{\partial \phi'_{2D}}{\partial t'} = -\nabla'^2_{2D} \phi'_{2D} + \nu |\psi'_{2D}|^2 \phi'_{2D} - E'_z \phi'_{2D}. \quad (4.3.5b)$$

These equations constitute the working form of the equations used in all subsequent analytical and numerical simulations.

Here

$$\kappa = \frac{2m\chi_{2D}}{\hbar^2}, \quad \tau = \frac{m_i}{m}, \quad \text{and} \quad \nu = \frac{m_i\chi_{2D}}{mg_{2D}} \quad (4.3.6)$$

are the dimensionless independent parameters. Physically, κ characterises the

back-action of the impurity on the condensate density, quantifying the extent of impurity-induced depletion. The parameter ν controls the strength of the condensate-mediated effective potential experienced by the impurity. The parameter τ sets the relative inertia of the impurity with respect to the condensate and therefore determines the separation of dynamical time scales between the two components. Finally

$$E'_z = \frac{2m_i\xi^2}{\hbar^2}E_z \quad (4.3.7)$$

represents the dimensionless energy of the impurity due to the z -confinement and the presence of the condensate. With this scaling, the conserved particle numbers become

$$N'_\psi = \int |\psi'_{2D}|^2 dV' = V', \quad (4.3.8a)$$

$$N'_\phi = \int |\phi'_{2D}|^2 dV' = 1. \quad (4.3.8b)$$

reflecting unit bulk density for the condensate and a unity-normalised impurity wavefunction.

The dimensionless system eqs. (4.3.5) conserves the following quantities:

Total energy:

$$E_{GC} = \int \left[|\nabla' \psi'_{2D}|^2 + \frac{1}{2} |\psi'_{2D}|^4 + \kappa |\psi'_{2D}|^2 |\phi'_{2D}|^2 + \frac{1}{\tau} |\nabla' \phi'_{2D}|^2 + \frac{\nu}{\tau} |\psi'_{2D}|^2 |\phi'_{2D}|^2 + \frac{E'_z}{\tau} |\phi'_{2D}|^2 \right] dV'. \quad (4.3.9)$$

Linear momentum:

$$\mathbf{P}' = \int \text{Im} \left(\psi'^*_{2D} \nabla' \psi'_{2D} + \frac{1}{\tau} \phi'^*_{2D} \nabla' \phi'_{2D} \right) dV', \quad (4.3.10)$$

Angular momentum (in 2D):

$$L'_z = \int \text{Im} \left(\psi'^*_{2D} (x' \partial_{y'} - y' \partial_{x'}) \psi'_{2D} + \frac{1}{\tau} \phi'^*_{2D} (x' \partial_{y'} - y' \partial_{x'}) \phi'_{2D} \right) dV'. \quad (4.3.11)$$

These conserved quantities provide useful diagnostics for the accuracy of numerical integrations and the interpretation of impurity dynamics within the dimensionless Gross–Clark framework.

Table 4.1 shows that experimentally relevant Bose-impurity mixtures span both weak and intermediate impurity-condensate coupling regimes. In particular, the wide variation in κ and ν allows controlled exploration of impurity localisation, while the mass ratio τ determines the relative dynamical response of the impurity compared to the condensate background [26, 58, 39, 1]. For completeness, the corresponding three-dimensional parameter estimates (without the tight z -confinement) are also shown; see Appendix A.3 for further details on the three-dimensional version of the dimensionless Gross-Clark model.

Mixture	Masses [kg]	Scatt. lengths	a_z, a_i [m]	ρ_{3D}, ρ_{2D}	$\kappa_{3D}, \nu_{3D}, \tau_{3D}$	$\kappa_{2D}, \nu_{2D}, \tau_{2D}$
$^{23}\text{Na} - ^{39}\text{K}$	$m_{\text{Na}} = 3.82 \times 10^{-26}$ $m_{\text{K}} = 6.47 \times 10^{-26}$	$a_{\text{NaNa}} = 52 a_0$ $a_{\text{NaK}} = 20\text{--}50 a_0$	$a_z = 1.72 \times 10^{-6}$ $a_i = 1.16 \times 10^{-6}$	$\rho_{3D} \approx 3 \times 10^{20}$ $\rho_{2D} \approx 1.6 \times 10^{10}$	$\kappa_{3D} = 0.19\text{--}0.48$ $\nu_{3D} = 1.03\text{--}2.59$ $\tau_{3D} = 1.70$	$\kappa_{2D} = 0.011\text{--}0.029$ $\nu_{2D} = 1.26\text{--}3.16$ $\tau_{2D} = 1.70$
$^{174}\text{Yb} - ^7\text{Li}$	$m_{\text{Yb}} = 2.89 \times 10^{-25}$ $m_{\text{Li}} = 1.16 \times 10^{-26}$	$a_{\text{YbYb}} = 105 a_0$ $a_{\text{YbLi}} = 21 \pm 3.2 a_0$	$a_z = 5.13 \times 10^{-7}$ $a_i = 8.97 \times 10^{-7}$	$\rho_{3D} \approx 3 \times 10^{20}$ $\rho_{2D} \approx 4 \times 10^{10}$	$\kappa_{3D} = 5.39$ $\nu_{3D} = 0.24$ $\tau_{3D} = 0.04$	$\kappa_{2D} = 0.48$ $\nu_{2D} = 0.18$ $\tau_{2D} = 0.04$
$^{87}\text{Rb} - ^{41}\text{K}$	$m_{\text{Rb}} = 1.44 \times 10^{-25}$ $m_{\text{K}} = 6.81 \times 10^{-26}$	$a_{\text{RbRb}} = 100 a_0$ $a_{\text{RbK}} = 250 a_0$	$a_z = 1.07 \times 10^{-6}$ $a_i = 1.30 \times 10^{-6}$	$\rho_{3D} \approx 1 \times 10^{19}$ $\rho_{2D} \approx 1.6 \times 10^{12}$	$\kappa_{3D} = 1.20$ $\nu_{3D} = 3.68$ $\tau_{3D} = 0.47$	$\kappa_{2D} = 0.35$ $\nu_{2D} = 3.35$ $\tau_{2D} = 0.47$
$^{23}\text{Na} - ^7\text{Li}$	$m_{\text{Na}} = 3.82 \times 10^{-26}$ $m_{\text{Li}} = 1.16 \times 10^{-26}$	$a_{\text{NaNa}} = 52 a_0$ $a_{\text{NaLi}} = 36 a_0$	$a_z = 1.23 \times 10^{-6}$ $a_i = 1.65 \times 10^{-6}$	$\rho_{3D} \approx 2 \times 10^{19}$ $\rho_{2D} \approx 2 \times 10^{12}$	$\kappa_{3D} = 0.24$ $\nu_{3D} = 0.90$ $\tau_{3D} = 0.30$	$\kappa_{2D} = 0.10$ $\nu_{2D} = 0.78$ $\tau_{2D} = 0.30$

Table 4.1: Estimated ranges of dimensionless parameters for various BEC–impurity systems [26, 58, 39, 1]. The subscripts “3D” refer to the case without tight confinement, whereas “2D” indicates the dimensionally reduced system.

4.4 Computing the Ground State Using the Imaginary-Time Method

The dynamical evolution of quantum systems depends sensitively on the choice of initial conditions [12]. Simulations are therefore usually initiated from a well-defined ground state. Analytical ground-state solutions exist only for simple cases, so numerical methods are generally required. Several numerical schemes have been developed for this purpose see e.g.[3, 55, 62] but for practicality and robustness, the imaginary-time propagation method is widely used. It provides a stable and accurate way to obtain the ground state, which serves as the initial condition for subsequent dynamical simulations[2, 12].

The ground state of the coupled Gross-Clark system, defined by Eqs. (4.3.5), is obtained numerically using the imaginary-time method (ITM). This method replaces the real time variable t' with an imaginary time $\tau'_{im} = -it'$, converting the governing equations into diffusion-type forms. In this formulation, high-energy components decay more rapidly, allowing the solution to converge to the lowest-energy stationary state of the system.

Applying the transformation $t' \rightarrow -i\tau'_{im}$ to Eqs. (4.3.5) gives

$$\frac{\partial \psi'_{2D}}{\partial \tau'_{im}} = \nabla_{2D}^2 \psi'_{2D} - (|\psi'_{2D}|^2 + \kappa |\phi'_{2D}|^2 - 1) \psi'_{2D}, \quad (4.4.1)$$

$$\tau \frac{\partial \phi'_{2D}}{\partial \tau'_{im}} = \nabla_{2D}^2 \phi'_{2D} - (\nu |\psi'_{2D}|^2 - E'_z) \phi'_{2D}. \quad (4.4.2)$$

These equations are parabolic and dissipative. When integrated in imaginary time, higher-energy modes are suppressed, and the system relaxes toward its ground state.

In practice, the condensate field ψ'_{2D} is evolved at a fixed chemical potential. This is equivalent to maintaining a constant average condensate density during the iteration, so that the overall normalisation of ψ'_{2D} remains unchanged. The

impurity field ϕ'_{2D} , on the other hand, is explicitly renormalised after each iteration to preserve the single-particle condition $\int |\phi'_{2D}|^2 d\mathbf{r}' = 1$. This ensures that the impurity contribution remains correctly normalised throughout the evolution.

Convergence is achieved when the relative change in E_{GC} and in both fields between successive iterations falls below a specified tolerance. The resulting stationary solutions $\psi'_{2D}(\mathbf{r}')$ and $\phi'_{2D}(\mathbf{r}')$ represent the ground state of the coupled system.

4.4.1 Numerical Implementation

Spatial derivatives in Eqs. (4.4.1) and (4.4.2) are evaluated using a Fourier pseudo-spectral discretisation on a uniform grid. Time stepping is performed with a Strang split-step scheme that alternates between the kinetic and nonlinear contributions [32]. After each propagation step, the impurity field ϕ'_{2D} is renormalised to unit norm, and the condensate field ψ'_{2D} is adjusted to maintain the fixed chemical potential. This approach is numerically stable and, in imaginary time, ensures a monotonic decrease in total energy, making it suitable for computing ground states of coupled (GC) systems.

At each iteration $\tau'_{im} \rightarrow \tau'_{im} + \Delta\tau'$, the following operations are applied:

1. Linear half-step (Fourier space):

$$\tilde{\psi}(k, \tau'_{im} + \frac{\Delta\tau'_{im}}{2}) = e^{-k^2 \Delta\tau'_{im}/2} \tilde{\psi}(k, \tau'_{im}), \quad (4.4.3)$$

$$\tilde{\phi}(k, \tau'_{im} + \frac{\Delta\tau'_{im}}{2}) = e^{-k^2 \Delta\tau'_{im}/(2\tau)} \tilde{\phi}(k, \tau'_{im}). \quad (4.4.4)$$

2. Nonlinear full-step (real space):

$$\psi'_{2D} \leftarrow \psi'_{2D} \exp[\Delta\tau'_{im}(1 - |\psi'_{2D}|^2 - \kappa|\phi'_{2D}|^2)], \quad (4.4.5)$$

$$\phi'_{2D} \leftarrow \phi'_{2D} \exp[-\Delta\tau'_{im}(\nu|\psi'_{2D}|^2)]. \quad (4.4.6)$$

3. **Renormalisation:** normalise ϕ'_{2D} to satisfy $\int |\phi'_{2D}|^2 d^2x = 1$; adjust ψ'_{2D} to enforce the prescribed chemical potential.
4. **Linear half-step (Fourier space):** repeat Step 1.

This iterative procedure progressively damps excited modes and converges to the stationary ground state of the coupled system. From this point on, we work exclusively with the effective two-dimensional description. For notational simplicity, the condensate and impurity fields are henceforth denoted by $\psi \equiv \psi'_{2D}$ and $\phi \equiv \phi'_{2D}$, respectively.

4.5 Summary

We introduced the Gross–Clark model, reduced it to a quasi–two–dimensional form under strong confinement, and non-dimensionalised it. The resulting framework identifies three dimensionless independent parameters κ , ν , and τ .

Chapter 5 uses this framework to determine the critical coupling for impurity self-localisation. Chapter 6 analyses impurity eigenstates in the core of a quantised vortex and their coupling to vortex structure.

Part II

Results and Analysis

Self-Localisation of a Single Impurity Field

This chapter studies the parameter range for which a single impurity field self-localises due to its nonlinear interaction with the condensate bulk. We begin with a variational (Gaussian) ansatz for the impurity wavefunction to obtain an analytic estimate of the localisation threshold. We then perform direct numerical simulations of the two-dimensional Gross–Clark equations to verify the validity of such a localisation threshold. We focus on a homogeneous condensate background without an external trapping potential, and on a periodic spatial system whose size is larger than the impurity localisation length scale. This isolates the self-localisation mechanism from boundary and trapping effects.

5.1 Introduction and Motivation

Impurity self-localisation in a Bose–Einstein condensate is a nonlinear effect in which a single impurity is trapped by its interaction with the surrounding condensate. It is related to phase separation in multicomponent condensates, but here localisation can occur even at vanishing impurity concentration.

Rica and Roberts [48] developed a coupled NLS/GPE model showing that several impurities can self-localise and even crystallise under suitable coupling; our dimensionless formulation reproduces their threshold phenomenology for a

single impurity. Studying a single impurity is useful for at least two reasons. First, it provides the simplest realisation of a Bose polaron, where the impurity is dressed by phonons of the condensate and may form a self-bound state. Second, the single-impurity threshold is a natural building block for understanding the collective behaviour of many impurities.

Our analysis extends the work by formulating the problem in the Gross–Clark framework introduced in Chapter 4, allowing for asymmetric impurity–condensate couplings κ and ν , and by constructing a full numerical phase diagram in two dimensions that can be directly compared with our variational prediction.

5.2 Model Setup

To investigate impurity self trapping in a Bose-Einstein condensate (BEC), we begin from the coupled dimensionless equations following the Gross-Clark model (4.3.5). For consistency with Chapter 4, we denote the condensate and impurity fields by ψ and ϕ , respectively.

The coupled Gross-Clark equations are governed by several dimensionless parameters. The parameters $\kappa > 0$ and $\nu > 0$ represent the impurity-condensate and condensate-impurity coupling strengths, respectively, introducing asymmetry between the two interaction channels. Specifically, κ controls depletion of the condensate by the impurity, while ν controls the strength of the resultant attractive potential felt by the impurity. The mass ratio is given by $\tau > 0$, and E'_z is a constant impurity offset. The case $\nu = \kappa$ reduces to the symmetric model considered by Rica and Roberts [48].

We treat ν and κ as independent parameters (asymmetric model). For a weak impurity perturbation, the condensate remains close to its homogeneous bulk

value $\psi = 1$ in the chosen dimensionless units, and may be written as

$$\psi = 1 - u, \quad |u| \ll 1. \quad (5.2.1)$$

The function u represents the local depletion of the condensate density induced by the impurity. This linearisation assumes that the impurity-induced depletion remains small, $|u(r)| \ll 1$, so that higher-order terms in u can be neglected. In Sec. 5.3 we verify a posteriori that this condition is reasonably satisfied in the parameter regime relevant to the localisation threshold. Substituting (5.2.1) into (4.3.5a) and linearising in u gives the inhomogeneous Helmholtz equation

$$(-\nabla^2 + 2)u = \kappa |\phi|^2. \quad (5.2.2)$$

This describes the condensate deformation $u(\mathbf{r})$ induced by the impurity density.

The Green's function $G_\alpha(\mathbf{r})$ of the operator $(-\nabla^2 + \alpha^2)$ in two spatial dimensions satisfies

$$(-\nabla^2 + \alpha^2)G_\alpha(\mathbf{r}) = \delta(\mathbf{r}), \quad (5.2.3)$$

where $\mathbf{r} = (x, y)$. By rotational symmetry the Green's function depends only on the radial distance $r = |\mathbf{r}|$, and in two dimensions is given by

$$G_\alpha(r) = \frac{1}{2\pi} K_0(\alpha r). \quad (5.2.4)$$

where K_0 is the modified Bessel function of the second kind. Setting $\alpha = \sqrt{2}$ yields

$$u(\mathbf{r}) = \frac{\kappa}{2\pi} \int K_0(\sqrt{2}|\mathbf{r} - \mathbf{r}'|) |\phi(\mathbf{r}')|^2 d^2 r'. \quad (5.2.5)$$

Here $\mathbf{r}$ denotes the observation point and $\mathbf{r}'$ the integration variable.

The perturbation therefore decays exponentially with the unity of the healing length.

Because $|\psi|^2 = (1 - u)^2 \simeq 1 - 2u$, an impurity that couples to condensate density

with strength ν experiences the induced potential

$$V_{\text{eff}}(\mathbf{r}) = -2\nu u(\mathbf{r}) = -\frac{\nu\kappa}{\pi} \int K_0(\sqrt{2}|\mathbf{r} - \mathbf{r}'|) |\phi(\mathbf{r}')|^2 d^2r'. \quad (5.2.6)$$

The condensate thus mediates an attractive interaction proportional to the product $\nu\kappa$ of the asymmetric couplings.

Substituting the effective potential (5.2.6) into the impurity Gross–Clark energy functional

$$E_\phi = \int d^2r [\tau |\nabla\phi|^2 + \nu |\psi|^2 |\phi|^2], \quad (5.2.7)$$

and including a factor of 1/2 to avoid double counting, yields the effective impurity energy functional

$$E_{\text{eff}} = \tau \int |\nabla\phi|^2 d^2r - \frac{\nu\kappa}{2\pi} \iint |\phi(\mathbf{r})|^2 K_0(\sqrt{2}|\mathbf{r} - \mathbf{r}'|) |\phi(\mathbf{r}')|^2 d^2r d^2r'. \quad (5.2.8)$$

The first term represents the kinetic or “surface-tension” cost of localisation, and the second encodes the condensate-mediated attraction.

A convenient trial function is the normalised Gaussian

$$\phi(\mathbf{r}) = \sqrt{\frac{N_\phi}{\pi\sigma^2}} \exp\left(-\frac{r^2}{2\sigma^2}\right), \quad (5.2.9)$$

where $N_\phi = \int |\phi|^2 d^2r$ is the conserved impurity norm and σ is a variational width. Then the kinetic contribution evaluates to

$$\int |\nabla\phi|^2 d^2r = \frac{N_\phi}{2\sigma^2}. \quad (5.2.10)$$

Exact Evaluation of the Interaction Term Let $\rho(\mathbf{r}) = |\phi(\mathbf{r})|^2$. Using the two-dimensional Fourier transform $\widehat{f}(\mathbf{k}) = \int e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) d^2r$,

$$\widehat{\rho}(\mathbf{k}) = N_\phi e^{-(\sigma^2 k^2)/4}, \quad \widehat{G_{\sqrt{2}}}(\mathbf{k}) = \frac{1}{k^2 + 2}.$$

Parseval's theorem yields

$$\iint \rho(\mathbf{r}) G_{\sqrt{2}}(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') d^2r d^2r' = \frac{1}{(2\pi)^2} \int \frac{|\widehat{\rho}(\mathbf{k})|^2}{k^2 + 2} d^2k. \quad (5.2.11)$$

After angular integration this reduces to

$$J(a) = \int_0^\infty \frac{k e^{-ak^2}}{k^2 + 2} dk,$$

with $a = \sigma^2/2$. Employing the standard identity

$$\int_0^\infty \frac{k e^{-ak^2}}{k^2 + \beta^2} dk = \frac{1}{2} e^{a\beta^2} E_1(a\beta^2),$$

where $E_1(x) = \int_x^\infty e^{-t} \frac{dt}{t}$ is the exponential integral function, and for large x $e^x E_1(x) \sim 1/x$. By setting $\beta^2 = 2$, gives the exact result

$$\boxed{\iint |\phi|^2 K_0(\sqrt{2}|\mathbf{r} - \mathbf{r}'|) |\phi|^2 d^2r d^2r' = \frac{N_\phi^2}{4\pi} e^{\sigma^2} E_1(\sigma^2).} \quad (5.2.12)$$

Variational Energy and Threshold Substituting (5.2.10) and (5.2.12) into (5.2.8) gives

$$\boxed{E_{\text{eff}}(\sigma) = \frac{\tau N_\phi}{2\sigma^2} - \frac{\nu \kappa N_\phi^2}{4\pi} e^{\sigma^2} E_1(\sigma^2).} \quad (5.2.13)$$

For large σ , we use the asymptotic form $e^{\sigma^2} E_1(\sigma^2) \simeq 1/\sigma^2$, which is accurate when σ exceeds the condensate healing length. Near the localisation threshold the optimal σ obtained from the variational energy is indeed of this order. We therefore expect the resulting critical condition to be quantitatively approximate but qualitatively reliable. The energy then simplifies to

$$E_{\text{eff}}(\sigma) \simeq \frac{1}{\sigma^2} \left[\frac{\tau N_\phi}{2} - \frac{\nu \kappa N_\phi^2}{4\pi} \right]. \quad (5.2.14)$$

A localised state forms when the coefficient of $1/\sigma^2$ becomes negative, yielding the critical condition

$$\boxed{(\nu \kappa)_c = \frac{2\pi\tau}{N_\phi}.} \quad (5.2.15)$$

The appearance of the product $\nu\kappa$ reflects the two-step mechanism underlying self-localisation: the impurity first depletes the condensate with strength set by κ , and the condensate deformation then acts back on the impurity with strength set by ν . The threshold therefore depends only on $\nu\kappa$, rather than on κ and ν separately.

In the symmetric limit $\nu = \kappa$, this reduces to

$$\boxed{\kappa_c^2 = \frac{2\pi\tau}{N_\phi}}, \quad (5.2.16)$$

which reproduces the Rica-Roberts threshold for self-trapping in two dimensions [48].

The criterion (5.2.15) expresses the balance between the kinetic spreading tendency of the impurity and the condensate-mediated attraction proportional to $\nu\kappa$. Below the threshold $(\nu\kappa) < (\nu\kappa)_c$ the impurity remains delocalised, whereas for $(\nu\kappa) > (\nu\kappa)_c$ a bound, self-trapped state appears.

5.3 Numerical Analysis of Self-Localisation

The numerical simulations are performed using the imaginary-time relaxation described in Section 4.4 of the dimensionless Gross-Clark equations to find the steady-state solution $\Psi = (\psi, \phi)$. The numerical results confirm the analytically predicted critical condition for self-trapping based on the product of the coupling constants $\nu\kappa$.

5.3.1 Analytic Threshold Calculation

To compare the numerical results with the derived variational threshold, we first calculate the critical product $(\nu\kappa)_c$. In all simulations in this chapter we fix the impurity mass ratio to $\tau = 1.0$ and the impurity norm to $N_\phi = 1.0$, so the analytic

threshold reduces to

$$(\nu\kappa)_c = \frac{2\pi\tau}{N_\phi} = \frac{2\pi(1.0)}{1.0} \approx 6.283 \quad (5.3.1)$$

Thus, the analytical phase boundary is the line where $\nu\kappa = 2\pi$, or $\kappa = 2\pi/\nu$.

We emphasise that this value is obtained within the Gaussian variational approximation and the large σ limit of the nonlocal interaction; it should therefore be viewed as an approximate benchmark for the full numerical simulations presented below.

5.3.2 Simulation Setup and Diagnostics

We solve the coupled Gross–Clark equations in imaginary time on a square domain $L_x = L_y = 120$ using a uniform grid of $N_x = N_y = 256$ points and periodic boundary conditions. The equations are discretised using a split-step Fourier method with time step $\Delta\tau = 5 \times 10^{-3}$ and a maximum of 2×10^5 steps. After each step, we renormalise the impurity wave function to keep N_ϕ fixed and fix the background condensate density by chemical potential (here set to unity). Convergence is monitored by the relative change of the total energy and of the wavefunctions. We stop the evolution when both change by less than 10^{-3} between consecutive time steps.

The phase of the system (Localised or Delocalised) is determined by two robust metrics measured at the end of the imaginary-time relaxation:

1. **Inverse Participation Ratio (IPR):** The inverse participation ratio of the impurity is defined as

$$IPR = \frac{\int |\phi(r)|^4 d^2r}{(\int |\phi(r)|^2 d^2r)^2} \quad (5.3.2)$$

which takes values of order $1/A$ for a delocalised state spread uniformly over the area $A = L_x L_y$ and becomes much larger when the impurity localises. In

practice we therefore use the dimensionless quantity $IPR \cdot A$ to distinguish between the two regimes.

2. Root-Mean-Square (RMS) Width (σ_ϕ): Defined as the standard deviation of the impurity density $|\phi|^2$, this serves as a measure of the impurity's physical size and defined by

$$\sigma_\phi^2 = \frac{\int |r - \langle r \rangle|^2 |\phi(r)|^2 d^2r}{\int |\phi(r)|^2 d^2r} \quad \langle r \rangle = \frac{\int r |\phi(r)|^2 d^2r}{\int |\phi(r)|^2 d^2r} \quad (5.3.3)$$

The combined numerical criterion for localisation is:

$$\text{Localised} \iff (IPR \cdot A \geq c_{IPR}) \quad \text{AND} \quad \left(\frac{\sigma_\phi}{\min(L_x, L_y)} \leq c_\sigma \right) \quad (5.3.4)$$

To classify the impurity state as localised or delocalised, we introduce the two diagnostic thresholds, c_{IPR} and c_σ . Based on inspection of the impurity profiles across the (κ, ν) plane, we choose $c_{IPR} = 9$ and $c_\sigma = 0.17$: states with $IPR \cdot A \geq c_{IPR}$ and $\sigma_\phi / \min(L_x, L_y) \leq c_\sigma$ are deemed localised, whereas those with $IPR \cdot A \leq c_{IPR}$ and $\sigma_\phi / \min(L_x, L_y) \geq c_\sigma$ are deemed delocalised. We have checked that varying these thresholds within a reasonable range ($c_{IPR} \in [7, 11]$, $c_\sigma \in [0.15, 0.20]$) shifts the phase boundary only slightly and does not change the overall agreement with the analytic prediction $\nu\kappa = 2\pi$.

We have performed basic convergence checks with respect to the system size and grid resolution. Increasing the box to $L_x = L_y = 160$ and the grid to $N_x = N_y = 256$, while keeping all other parameters fixed, leads to changes of less than a few percent in the critical product $\nu\kappa$ extracted from our diagnostics. This indicates that finite-size and discretisation effects do not qualitatively affect the localisation threshold.

5.3.3 Visualization and Agreement

The agreement between the simulation results and the analytic theory is presented in a two-part visualization.

Continuous Metric Heatmap (σ_ϕ)

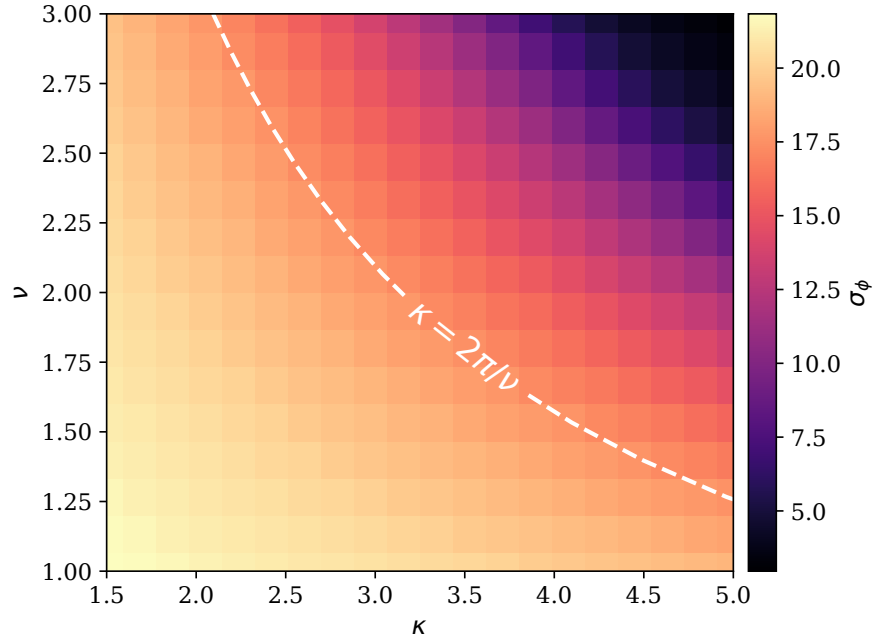


Figure 5.3.1: The colour map shows the steady state RMS width σ_ϕ across the (κ, ν) parameter space, ranging from delocalised (light yellow, high σ_ϕ) to localised (dark purple, low σ_ϕ). The white dashed line represents the analytic critical threshold, $\kappa = 2\pi/\nu$.

The continuous heatmap of the RMS width, σ_ϕ , across the (κ, ν) parameter space in Fig. 5.3.1 clearly shows the transition boundary.

- **Delocalised Region (High σ_ϕ):** In the weak-coupling regime the impurity spreads over a significant fraction of the system, resulting in a large RMS width σ_ϕ .
- **Localised Region (Low σ_ϕ):** In the strong-coupling regime the impurity forms a tightly bound state, for which σ_ϕ is small compared to the system

size.

The theoretical boundary $\kappa = 2\pi/\nu$ (represented by the white dashed line in Figure 5.3.1) accurately traces the sharp transition in the numerical metric, demonstrating strong quantitative agreement.

Binary Phase Map

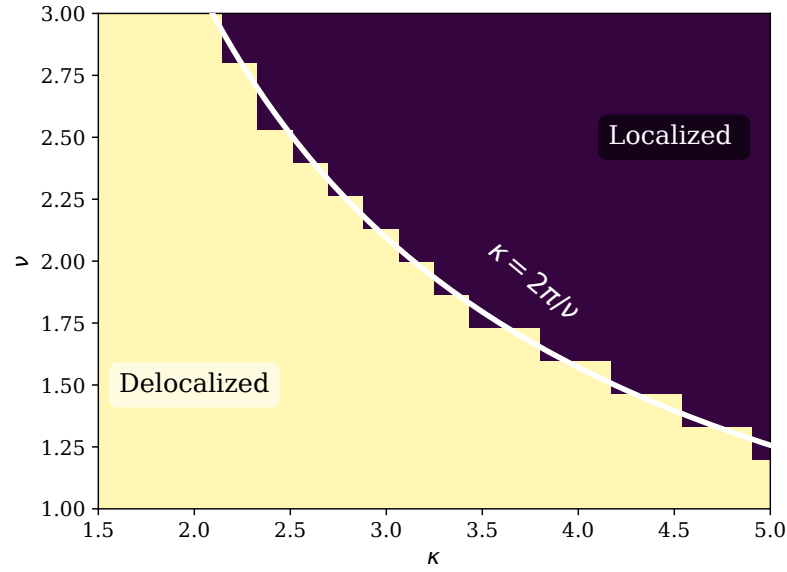
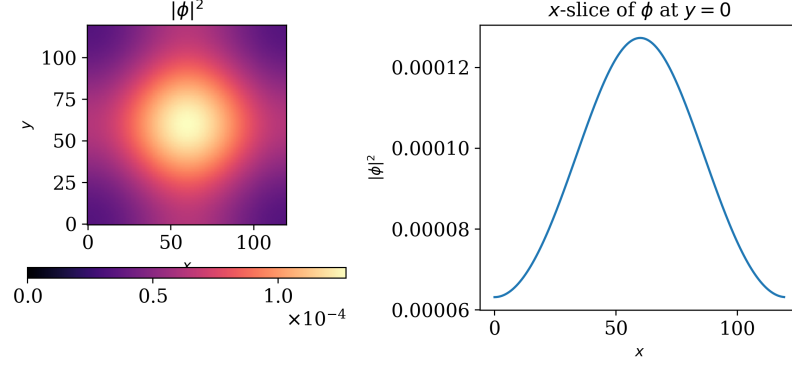


Figure 5.3.2: The map shows the numerical classification of the impurity state (Localised/Delocalised) across the (κ, ν) parameter space. The smooth white line represents the analytical critical threshold, $\kappa = 2\pi/\nu$.

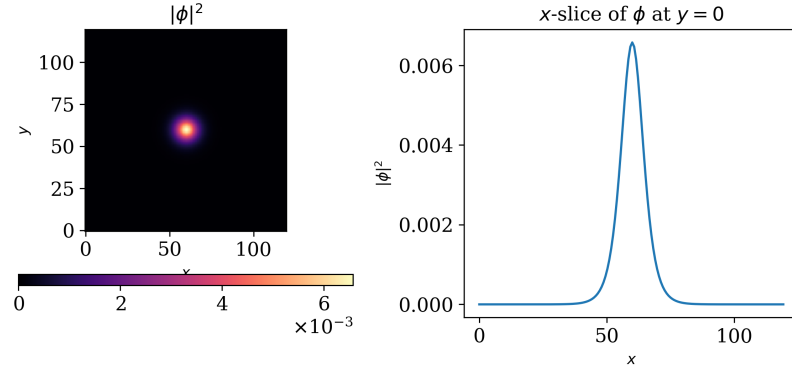
The binary phase map (Figure 5.3.2) compares the discrete numerical classification (staircase background) with the smooth analytical boundary. The staircase boundary of the numerical result follows the smooth analytic curve closely, with the majority of simulated points classified as **Localised** only when $\nu\kappa$ exceeds the theoretical threshold of 2π . This visually confirms that the self-trapping mechanism is governed by the product of the asymmetric coupling constants, $\nu\kappa$.

While Fig. 5.3.1 highlights the continuous behaviour of the RMS width σ_ϕ , Fig. 5.3.2 shows a binary phase diagram constructed using both the inverse

participation ratio (IPR) and the RMS width as localization diagnostics. The agreement between these independent numerical measures ensures a robust classification of the localized phase. The resulting phase boundary closely follows the analytical prediction, $\kappa = 2\pi/\nu$.



(a) Delocalised State ($\nu = 1.0, \kappa = 2.0$)



(b) Localised State ($\nu = 3.0, \kappa = 4.0$)

Figure 5.3.3: The final steady-state solutions for the impurity wave function ϕ (density $|\phi|^2$, and 1D cross section at $y = 0$) taken from the parameter space. (a) Delocalised Phase ($\nu\kappa = 2.0 < 2\pi$): The impurity density is low and spread uniformly across the domain. (b) Localised Phase ($\nu\kappa = 12.0 > 2\pi$): The impurity collapses into a self-trapped solitary structure with a high-density, Gaussian-like peak.

Figure 5.3.3 compares impurity steady states below and above the predicted threshold. Panel (a) ($\nu = 1.0, \kappa = 2.0$); ($\nu\kappa = 2.0 < 2\pi$) shows a delocalised impurity: the density is broad and the ($y = 0$) cross-section is wide and low. Panel (b) ($\nu = 3.0, \kappa = 4.0$); ($\nu\kappa = 12.0 > 2\pi$) shows a localised state: the density concentrates near the centre and the ($y = 0$) slice exhibits a narrow, high peak. These observations are consistent with the criterion ($\nu\kappa > 2\pi$) for

self-trapping.

5.4 Summary

This chapter established the critical condition for the self-localisation of a single impurity field within a two-dimensional Bose-Einstein condensate governed by the Gross-Clark model.

The analytical derivation, based on a Gaussian variational ansatz, yielded an effective energy functional that explicitly balanced the kinetic spreading of the impurity with the attractive potential mediated by the condensate. This analysis identified the critical threshold for self-trapping as the product of the coupling constants: $(\nu\kappa)_c = 2\pi\tau/N_\phi$.

Direct numerical simulations performed across the (ν, κ) parameter space confirmed this theoretical prediction with high accuracy. The transition from a delocalised, spread-out state ($\nu\kappa < 2\pi$) to a tightly bound, localised state ($\nu\kappa > 2\pi$) was clearly mapped using two independent diagnostics: the Inverse Participation Ratio and the Root-Mean-Square width (σ_ϕ). The strong quantitative agreement between the numerical phase boundary and the analytical line $\nu\kappa = 2\pi$ confirms that the self-trapping mechanism is universally governed by the product of the asymmetric coupling strengths, $\nu\kappa$.

Eigenstates of an impurity trapped in a two-dimensional quantised vortex

Building on the self-localisation analysis of Chapter 5, this chapter investigates the eigenstates of an impurity confined in the core of quantised vortex. Using the Gross–Clark model in the quasi-two-dimensional limit, we develop an iterative numerical algorithm that alternates imaginary-time propagation for the condensate with an eigensolver for the impurity. This approach yields self-consistent stationary states characterised by two independent parameters and allows us to study impurity localisation within vortex cores, the dependence on circulation quanta, and the back-action of the impurity on the vortex density profile.

The chapter is organised as follows. Section 6.1 sets out the model. Section 6.2 explains how to obtain the ground-state solution for the coupled impurity and Bose-Einstein condensate (BEC). Section 6.3 presents the iterative numerical algorithm. Section 6.4 contains the numerical results and their physical interpretation, focusing primarily on the impurity localised ground and excited states.

6.1 Model setup

The aim of this chapter is to study the two-dimensional eigenstates of an impurity trapped in the core of a quantised BEC vortex. We start from the dimensionless Gross-Clark equations (4.3.5), which couple the condensate wave function ψ and the impurity field ϕ in the quasi-two-dimensional limit. To describe a single vortex at the origin, we switch from Cartesian coordinates (x, y) to polar coordinates (r, θ) , with $x = r \cos \theta$ and $y = r \sin \theta$.

Stationary vortex impurity states are taken in the form

$$\begin{aligned}\psi(r, \theta, t) &= f(r) e^{is\theta}, \\ \phi(r, \theta, t) &= g(r) \exp\left[i\left(\ell\theta - \frac{E-E_z}{\tau}t\right)\right],\end{aligned}\tag{6.1.1}$$

where $f(r)$ and $g(r)$ are the real radial profiles of the condensate and impurity, respectively. The integer $s \in \mathbb{Z}$ is the winding number of the quantised vortex, while $\ell \in \mathbb{Z}$ denote the angular momentum quantum number. The dimensionless energy of the impurity eigenstate is E and E_z is the constant energy offset arising from the frozen axial degree of freedom introduced in Chapter 4 [7]. The condensate field ψ carries no explicit time dependence apart from the global phase fixed by the chemical potential.

Because the trapping potential and the vortex at the origin are cylindrically symmetric, the condensate and impurity densities depend only on the radial coordinate (r) . The full angular dependence is carried by the phase factors $(e^{is\theta})$ and $(e^{i\ell\theta})$, so the radial profiles $(f(r))$ and $(g(r))$ depend only on (r) and not on (θ) .

Substituting the ansatz (6.1.1) into the dimensionless Gross-Clark equations (4.3.5), reduces the problem to a pair of coupled radial ordinary differential equations (ODEs) for the radial profiles $f(r)$ and $g(r)$:

$$\frac{d^2 f}{dr^2} + \frac{1}{r} \frac{df}{dr} - \left(\frac{s^2}{r^2} + f^2 + \kappa g^2 - 1 \right) f = 0 \tag{6.1.2a}$$

$$\frac{d^2 g}{dr^2} + \frac{1}{r} \frac{dg}{dr} - \left(\frac{\ell^2}{r^2} + \nu f^2 \right) g = E g \quad (6.1.2b)$$

Equation (6.1.2a) determines the condensate vortex profile, including the back-action of the impurity through the κg^2 term. Equation (6.1.2b) is the impurity eigenvalue problem in the vortex background, where νf^2 acts as an effective trapping potential. Together, these equations determine self-consistent impurity states confined in quantised vortex cores.

6.2 Ground-State Computation

To obtain the ground-state solution of the coupled Bose–Einstein condensate (BEC) and impurity system, we use the standard imaginary-time propagation method. For a given choice of chemical potential (here set to unity) which fixes the normalisation of $f(r)$ and a normalised impurity field $g(r)$, this method produces a self-consistent solution of the coupled nonlinear system, where the BEC profile $f(r)$ and impurity density $g(r)$ evolve simultaneously until convergence.

In practice, the radial equations (6.1.2) are evolved in imaginary time on a finite radial grid. Spatial derivatives are approximated using second-order finite differences. After each time step, the impurity field is renormalised to enforce

$$2\pi \int_0^{r_{\max}} r |g(r)|^2 dr = 1.$$

Convergence is assessed from the maximum relative change in successive iterations of f and g , together with the decrease of the impurity energy.

Figure 6.2.1 shows the ground state of the condensate–impurity system. Starting from an initial Gaussian impurity profile, the field $g(r)$ contracts towards the origin while the condensate density $f(r)$ relaxes to the expected bulk value of unity at large r . The impurity energy decreases monotonically during the evolution and stabilises once the system reaches its lowest energy configuration. The convergence of both fields and of the energy confirms that

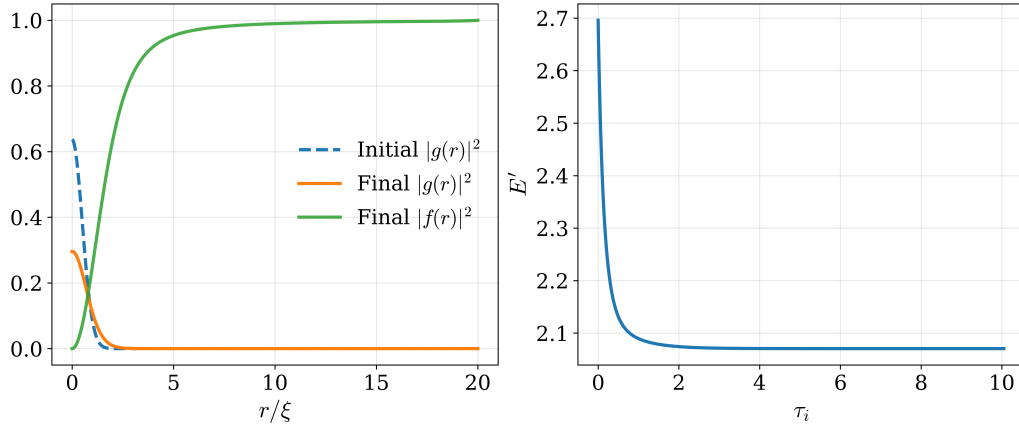


Figure 6.2.1: Ground-state computation of the coupled condensate-impurity system using imaginary-time propagation for fixed quantum numbers $s = 1$ and $\ell = 0$. Left: impurity density $|g(r)|^2$ at the initial and converged states, together with the converged condensate density $|f(r)|^2$. The impurity contracts towards the origin while the condensate adjusts to unit bulk density away from the centre. Right: convergence of the impurity energy $E(\tau_i)$ as a function of imaginary time τ_i , showing decrease at the ground state value.

the numerical scheme reliably finds the self-consistent ground state.

6.3 Numerical Methods for Steady-State Solutions

The main objective of this chapter is to go beyond the ground state and compute excited impurity states in the presence of a quantised vortex background. Since no analytical solutions are available for such excitations, we develop an iterative numerical scheme capable of accurately resolving both ground and excited states within the fully coupled impurity-BEC system. The scheme alternates between solving Eqs. (6.1.2a) and (6.1.2b) while holding g and f fixed, respectively. Equation (6.1.2a) is solved, keeping g fixed, by using the imaginary time approach allowing f to converge to its ground-state solution. On the other hand, keeping f fixed, eq. (6.1.2b) results simply in a linear eigenvalue problem: it is solved using standard numerical techniques, that allow us to find all the (localised and delocalised) eigenstates and their respective (energy) eigenvalues. We initialise this iterative algorithm by solving (6.1.2b) using a Padé ansatz for f [4], then selecting the desired eigenstate of g ,

and using it after appropriate normalisation (4.3.8b) to solve (6.1.2a). Repeating these steps until a chosen convergence threshold is met yields the steady-state solutions.

6.3.1 Iterative Numerical Scheme for Computing Impurity Eigenstates

Imaginary-Time Evolution for $f(r, \tau_{im})$: To obtain the stationary condensate profile $f(r)$ we evolve $f(r, \tau_{im})$ in imaginary time using relaxation of the dimensionless radial Gross–Pitaevskii equation:

$$\frac{\partial f}{\partial \tau_{im}} = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r} \frac{\partial f}{\partial r} - \left(\frac{s^2}{r^2} + f^2 + \kappa g^2 - 1 \right) f,$$

with the impurity wave function $g(r)$ held fixed during each update of f . Imaginary time projects the system towards a stationary state by damping higher energy modes.

We discretise the radial operator with second-order central finite differences on a uniform radial grid of spacing Δr , and integrate in τ_{im} with a fourth-order Runge–Kutta (RK4) scheme.

To impose physically appropriate boundary conditions for a singly quantised vortex, we enforce a Dirichlet condition ($f(0) = 0$), which ensures that the condensate density vanishes at the vortex core, and a Neumann condition ($\partial_r f|_{r=r_{\max}} = 0$), so that the profile approaches a flat background at the outer edge of the computational domain.

As an initial condition, we use the Padé approximation (2.6.5) for a singly quantised vortex [4], which provides an accurate analytic seed for the iterative method. Convergence is evaluated via a relative update criterion:

$$\Delta f = \frac{\sum_r |f^{\text{new}}(r) - f^{\text{old}}(r)|}{\sum_r |f^{\text{old}}(r)|},$$

In practice we choose ($\text{tol}_f = 10^{-6}$) for all simulations in this chapter, which is sufficient to ensure that further imaginary-time evolution does not change observables within numerical accuracy.

Matrix eigenvalue method for the impurity equation

The impurity bound states are computed by solving the radial Schrödinger eigenvalue problem:

$$\frac{\partial^2 g}{\partial r^2} + \frac{1}{r} \frac{\partial g}{\partial r} - \left(\frac{\ell^2}{r^2} + \nu f^2 \right) g = E g.$$

The term ℓ^2/r^2 is the centrifugal barrier, which grows with $\ell > 0$ and is absent when $\ell = 0$.

We discretise this equation using second-order central finite differences on the same uniform radial grid as for the condensate, $r_i = i\Delta r$ with spacing Δr where i is the radial grid index, which produces a sparse symmetric matrix eigenvalue problem:

$$A \mathbf{g} = E \mathbf{g} \tag{6.3.1}$$

Here $\mathbf{g}$ is the vector with components $g_i = g(r_i)$, and A is the sparse matrix representation of the radial kinetic plus potential operator.

On the discrete grid we collect the impurity values into a vector $\mathbf{g} = (g_0, \dots, g_{n-1})^T$. The matrix A is then an $n \times n$ sparse matrix acting on $\mathbf{g}$. In the formulas below we adopt Python-style zero-based indexing, so that the first and last grid points correspond to indices $i = 0$ and $i = n - 1$, respectively.

For interior grid points r_i (away from the boundaries), the second-order central finite-difference discretisation gives matrix elements

$$A_{i,i-1} = \frac{1}{\Delta r^2} - \frac{1}{2r_i \Delta r}, \quad A_{i,i} = -\frac{2}{\Delta r^2} + \frac{\ell^2}{r_i^2} + \nu f^2(r_i), \quad A_{i,i+1} = \frac{1}{\Delta r^2} + \frac{1}{2r_i \Delta r},$$

corresponding to the discretised operator $(\partial_r^2 + \frac{1}{r} \partial_r - (\ell^2/r^2 + \nu f^2))$.

The lowest eigenvalues and eigenvectors are obtained using sparse numerical solvers.

Because the radial operator contains singular terms proportional to $1/r$ and ℓ^2/r^2 , special care is required near the origin. We therefore treat the inner boundary at $r = 0$ separately.

Inner Boundary Condition at $r = 0$

Boundary conditions depend on ℓ :

- For $\ell = 0$, the wave function must be regular at the origin, satisfying $g'(0) = 0$. Since the grid begins at $r = \Delta r$, the value at the origin is reconstructed using a second-order forward finite-difference extrapolation:

$$g(0) = \frac{4g(\Delta r) - g(2\Delta r)}{3}. \quad (6.3.2)$$

This extrapolated value is used to evaluate the differential operator at the first grid point $r = \Delta r$, resulting in the matrix entries:

$$\begin{aligned} A_{0,0} &= \frac{2}{3\Delta r^2} + \frac{2}{3\Delta r \cdot r_1} + \nu f^2(r_1), \\ A_{0,1} &= -\left(\frac{2}{3\Delta r^2} + \frac{2}{3\Delta r \cdot r_1} \right), \end{aligned} \quad (6.3.3)$$

where $r_1 = \Delta r$.

- For $\ell > 0$, the centrifugal term ℓ^2/r^2 diverges at the origin, and the wave function must vanish therefore $g(0) = 0$. This condition is enforced directly by setting $g_0 = 0$. The matrix entries at $r = \Delta r$ are then constructed using standard finite differences:

$$\begin{aligned} A_{0,0} &= \frac{2}{\Delta r^2} + \nu f^2(r_1) + \frac{\ell^2}{r_1^2}, \\ A_{0,1} &= -\left(\frac{1}{\Delta r^2} + \frac{1}{2r_1 \Delta r} \right). \end{aligned} \quad (6.3.4)$$

Outer Boundary Condition at $r = r_{\max}$

For both $\ell = 0$ and $\ell > 0$, the wave function is required to vanish at large distances to ensure localisation. This is enforced via a Dirichlet boundary condition:

$$g(n-1) = 0.$$

At the final grid point $r = r_{n-1}$ the operator is evaluated using central finite differences, giving:

$$\begin{aligned} A_{n-1, n-2} &= \frac{1}{2r_{n-1}\Delta r} - \frac{1}{\Delta r^2}, \\ A_{n-1, n-1} &= \frac{2}{\Delta r^2} + \nu f^2(r_{n-1}) + \frac{\ell^2}{r_{n-1}^2}. \end{aligned} \tag{6.3.5}$$

In general, an impurity state can be written as a superposition $\sum_j c_j g_j(r)$, but here we focus on individual eigenstates. Therefore, after solving the matrix eigenvalue problem, we obtain a discrete set of impurity eigenstates labelled by a radial quantum number j for each angular momentum ℓ . The corresponding eigenvectors are denoted $g_j(r)$. Each eigenvector is normalised according to the two-dimensional integral:

$$2\pi \sum_{i=0}^{n-1} r_i |g_j(r_i)|^2 \approx 2\pi \int_0^{r_{\max}} dr \, r |g_j(r)|^2 = 1,$$

so that $(|g_j(r)|^2)$ represents the radial probability density of the j -th impurity eigenstate.

Convergence is verified by grid refinement: we increase the number of radial grid points n and check that the eigenvalues do not change appreciably. As shown in Figure 6.3.1, the first eight eigenvalues are stable for $n \gtrsim 10^3$, indicating proximity to the continuum limit across all ℓ .

Figure 6.3.2 summarises the self-consistent iterative loop used to solve the coupled radial equations (6.1.2) numerically. The detailed algorithm proceeds as follows:

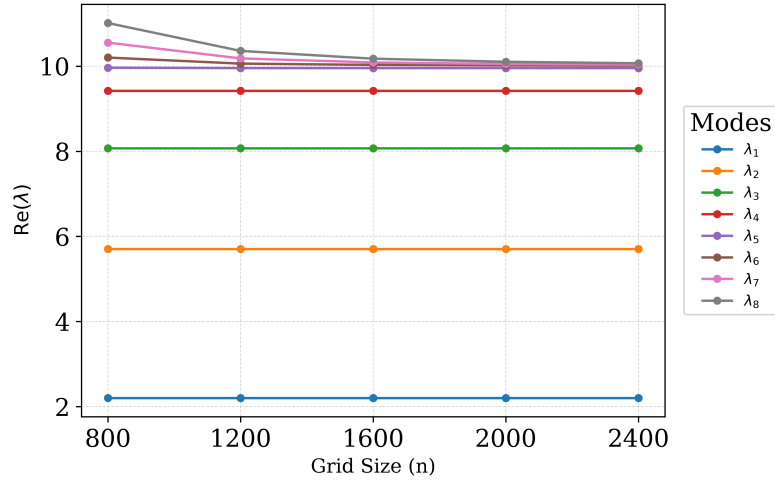


Figure 6.3.1: First eight eigenvalues as a function of the radial grid size n . Each coloured curve represents a different mode, and the flattening of each curve for larger n indicates that the eigenvalues converge once the grid resolution is sufficiently refined.

1. **Initial BEC.** The BEC profile $f(r)$ is initialised using the Padé approximation [4], providing a practical first guess for a singly quantised vortex.
2. **Initial impurity solution.** With the initial f held fixed, the impurity is diagonalised to find its eigenvectors and eigenvalues. The desired eigenvector g_j is selected and normalised according to

$$2\pi \int_0^{r_{max}} dr r |g_j(r)|^2 = 1.$$

3. Self-consistent loop.

- (a) Imaginary-time evolution of f : Propagate f in imaginary time with g_j fixed until the superfluid functional convergence criterion δf is satisfied.
- (b) Update impurity wave-function g : Solve again the linear eigenvalue problem with the updated f , selecting the same j th eigenstate as initially chosen, and re-normalise to obtain the updated impurity wave-function g_j^{new} .

(c) Check convergence: Evaluate the relative changes

$$\Delta f = \frac{\|f^{\text{new}} - f^{\text{old}}\|}{\|f^{\text{old}}\|}, \quad \Delta g = \frac{\|g_j^{\text{new}} - g_j^{\text{old}}\|}{\|g_j^{\text{old}}\|}.$$

The iteration stops when both relative changes satisfy $\max(\Delta f, \Delta g) < \text{tol}$; otherwise, set $(f^{\text{old}}, g_j^{\text{old}}) \leftarrow (f^{\text{new}}, g_j^{\text{new}})$ and repeat the loop.

This iterative method yields fully self-consistent stationary solutions $\{f(r), g(r)\}$ together with the corresponding impurity bound-state energies. Convergence is typically achieved after $\mathcal{O}(10^2 - 10^3)$ iterations, depending on the interaction parameters (κ, ν) and the numerical settings, including the grid resolution and time step. Throughout this chapter we use $\text{tol}_f = \text{tol}_g = 10^{-6}$, ensuring that further iterations modify the condensate and impurity densities, as well as the eigen-energies, by less than 10^{-4} in relative terms.

The radial coordinate is discretised on a uniform grid with spacing $\Delta r = 0.05$ using $n = 1000$ grid points, corresponding to a maximum radius $r_{\text{max}} = 50$. This domain size is chosen to be significantly larger than the vortex core and the spatial extent of all localised impurity states considered here. Convergence with respect to the domain size was verified by increasing r_{max} at fixed Δr , confirming that the profiles and eigenvalues of localised states are insensitive to the boundary, while delocalised states exhibit a clear dependence on r_{max} .

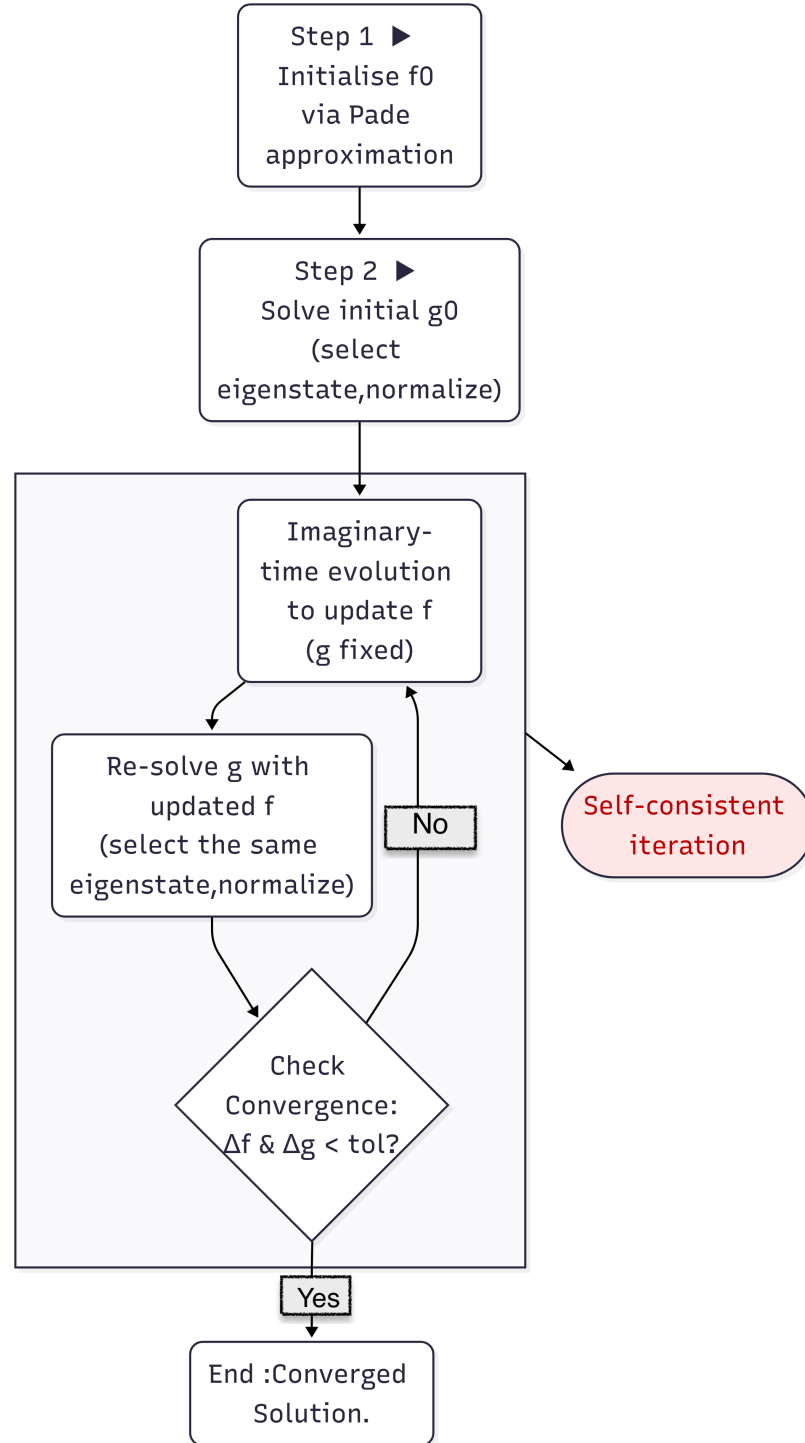


Figure 6.3.2: Flow diagram of the self-consistent algorithm used to obtain the impurity wave-function g in the vortex background f . The Padé profile is used to initialise the superfluid density; ; the two arrows in the shaded box illustrate the alternation between imaginary-time propagation of f (with g fixed) and recomputation of g (with f fixed) until convergence.

6.4 Results and analysis

Back-action and core broadening:

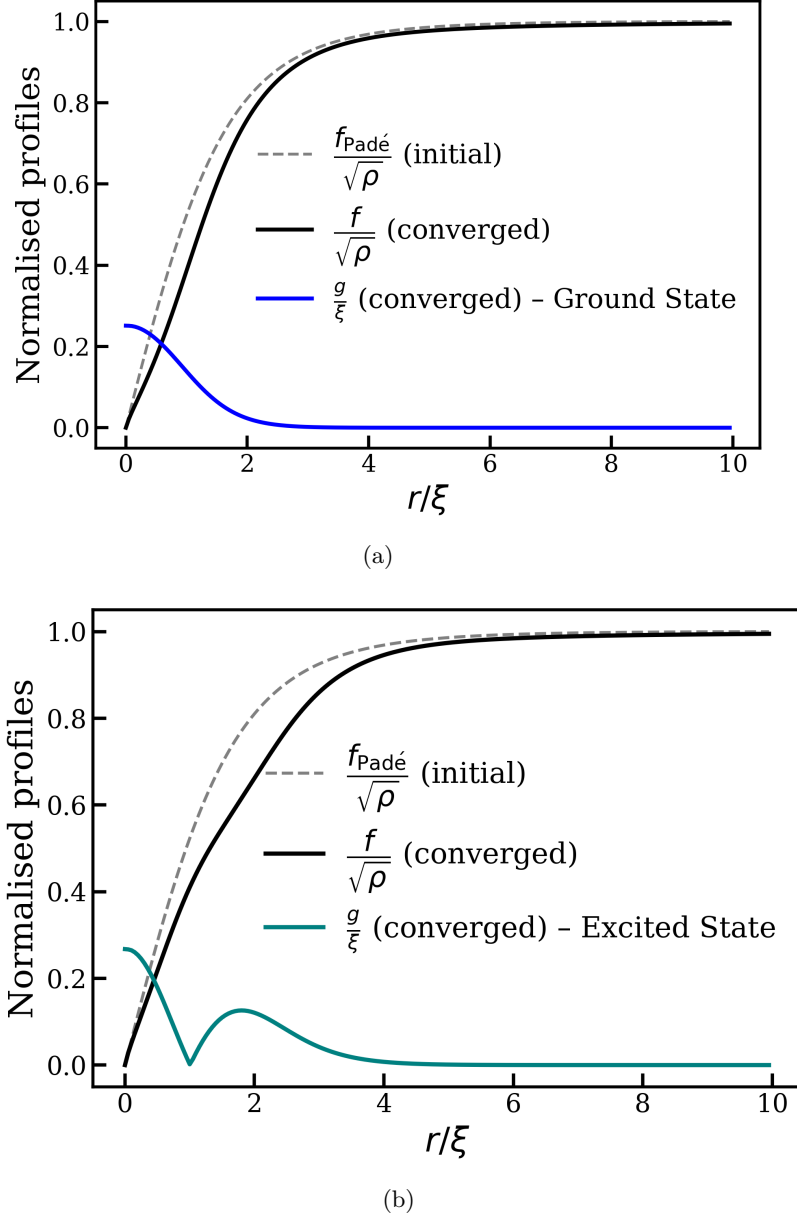


Figure 6.4.1: **Impurity back-action on the BEC vortex profile.** The dashed grey curve is the initial Padé approximation for the vortex density; the solid black curve is the converged BEC profile after self-consistent coupling to the impurity. **(a)** Ground-state impurity ($\kappa = \nu = 10$) produces a sharply localised $g_0(r)$ (blue) that widens the vortex core relative to the Padé guess. **(b)** First excited impurity state (teal) possesses one radial node and induces an even broader density depletion.

Figure 6.4.1 illustrates two examples of the steady-state solution achieved by the numerical algorithm for ($\kappa = 10$ and $\nu = 10$). As discussed in Chapter 5, the same parameters already produce a tightly localised impurity even in the absence of a vortex. Using the same values here ensures that any additional changes to the condensate profile can be attributed to the impurity–vortex coupling.

The blue curve in Fig. 6.4.1(a) represents the ground-state impurity wave function $g_0(r)$, which remains sharply peaked around the vortex centre and decays rapidly on the scale of a few healing lengths. The teal curve in Fig. 6.4.1(b) shows the first excited impurity state $g_1(r)$, which has a single radial node and a broader spatial extent; it crosses zero once before decaying towards the edge of the computational domain. In both panels the dashed grey line denotes the initial Padé approximation for the vortex condensate, while the solid black line is the converged BEC radial profile $f(r)$ obtained after coupling to the impurity.

A comparison between the dashed and solid black curves demonstrates that, for such values of κ and ν , the impurity whether in its ground or first excited state, broadens the vortex core relative to the Padé guess. This broadening reflects the nonlinear back-action of the impurity on the superfluid, and confirms the necessity of a fully coupled Gross-Clark treatment.

Localised vs delocalised states and the role of ν

We first define what we mean by localised and delocalised impurity eigenstates on the finite numerical domain. On the discrete radial grid, the derivative of the impurity wave function at the outer boundary $r = r_{\max}$ is approximated by

$$\left. \frac{dg}{dr} \right|_{r_{\max}} \approx \frac{g(r_{\max}) - g(r_{\max} - \Delta r)}{\Delta r}.$$

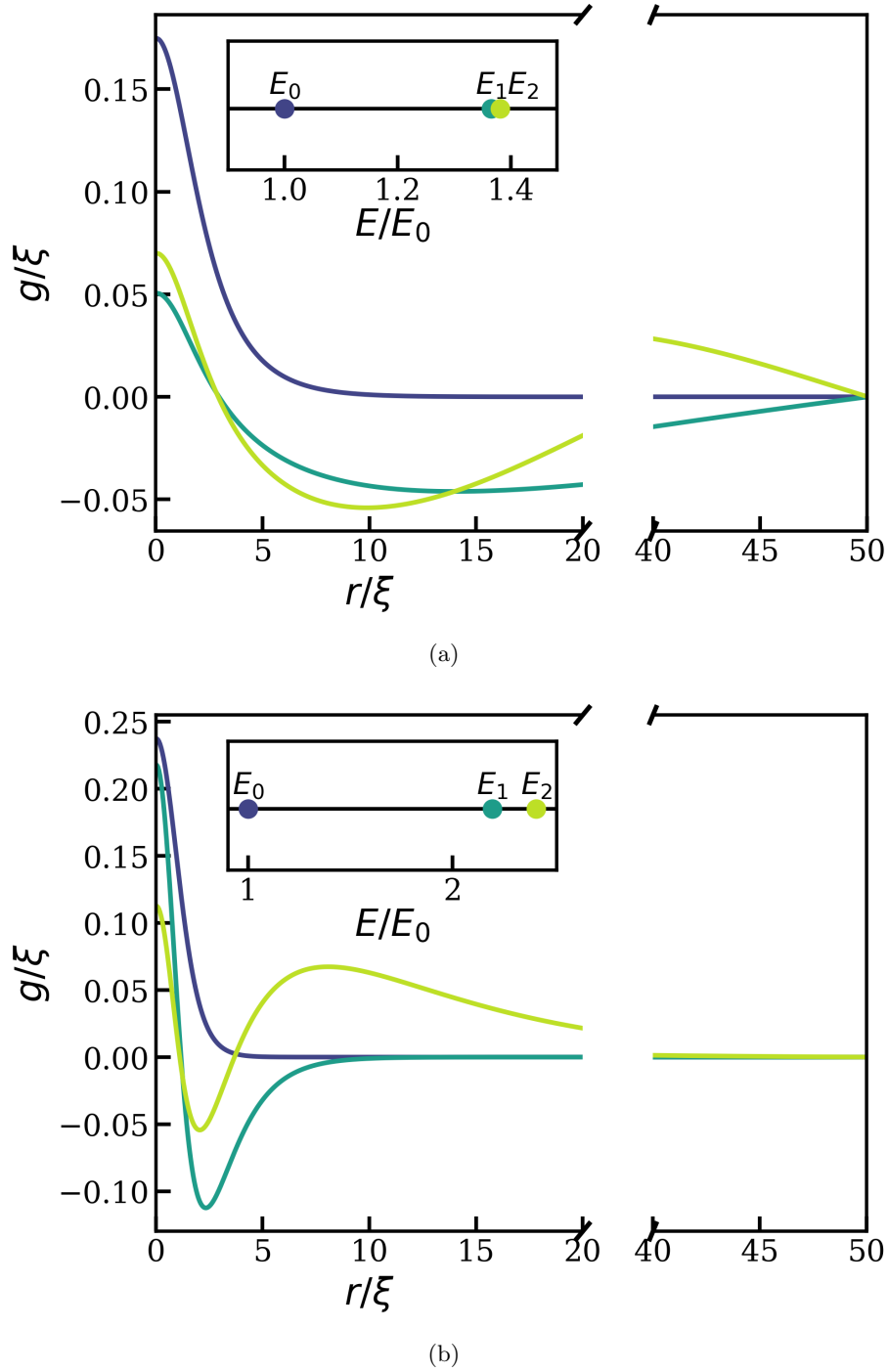


Figure 6.4.2: Impurity eigenstates for two interaction regimes. Insets show the corresponding eigen-energies E_j , with the discrete states E_0 , E_1 , E_2 marked. (a) Weaker coupling, $\kappa = 1, \nu = 1$: the effective potential is shallow, and higher eigenmodes remain finite as $r/\xi \rightarrow r_{\max}$, signalling delocalised impurity states. (b) Stronger coupling, $\kappa = 1, \nu = 5$: the impurity eigenmodes decay rapidly to zero at large radii, indicating tight localisation in the vortex core.

We then classify an eigenstate as localised if its radial derivative at the boundary is below a small numerical threshold

$$\left| \frac{dg}{dr}(r_{\max}) \right| < \varepsilon_{\text{loc}},$$

with $\varepsilon_{\text{loc}} = 10^{-4}$ in all simulations. On a finite computational domain, this condition provides a practical indicator of spatial confinement, since a genuinely bound state must decay sufficiently rapidly at large radii. States that fail this criterion are classified as delocalised. In practice, we find that localised states identified in this way are insensitive to moderate increases of the domain size, whereas delocalised states change noticeably when $r_{\max}$ is increased.

We now illustrate how the impurity eigenstates evolve between localised and delocalised regimes as the interaction parameters are varied. To isolate this effect, we keep the impurity back-action parameter fixed at $\kappa = 1$ and vary the effective potential strength ν .

Figure 6.4.2 shows representative eigenfunctions and eigen-energies for two such parameter choices. In panel (a) we consider a weaker effective confinement with $\kappa = 1$, $\nu = 1$. The effective potential in the vortex core is shallow, and while the lowest mode $g_0(r)$ remains peaked at the origin, higher modes extend over the whole domain and approach small, approximately constant values as $r/\xi \rightarrow r_{\max}$. These modes do not satisfy the localisation criterion above and are therefore classified as delocalised. In contrast, panel (b) corresponds to a stronger effective confinement with $\kappa = 1$, $\nu = 5$. Here all eigenmodes shown decay rapidly to zero at large radii and meet the localisation criterion, indicating tight localisation of the impurity in the vortex core.

The insets provide a complementary spectral view by showing the real eigen-energies E_j associated with the modes in each panel. As the potential is weakened, the lowest eigenvalue E_0 moves towards a cluster of higher-lying levels. All eigenvalues are real within numerical precision, as expected for the Hermitian radial eigenvalue problem. On a finite computational domain the

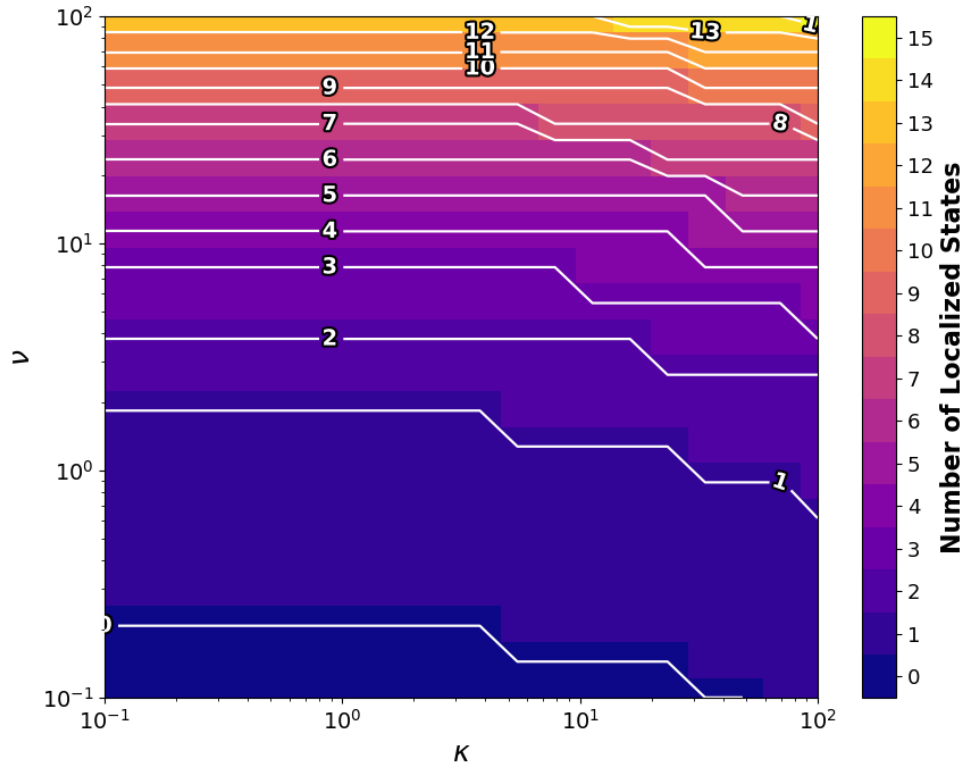


Figure 6.4.3: Number of localised impurity states as a function of the dimensionless couplings κ and ν . Log-log axes highlight the broad parameter range; contour labels give the integer state count. The ridge between 0 and 1 indicates the localisation threshold for the ground state.

exact position of the continuum threshold is not known, but the accumulation of eigenvalues into a dense set at higher energies is the numerical signature of the onset of the continuum band. Taken together, the spatial behaviour of the eigenfunctions and the eigenvalue clustering in Fig. 6.4.2 support the classification of the states in panel (a) as delocalised and those in panel (b) as localised.

State count across parameter space:

Figure 6.4.3 maps the total number of localised impurity bound states (colour scale and contour labels) as a function of the dimensionless parameters κ and ν . Increasing ν at fixed κ deepens the effective potential experienced by the impurity, leading to additional bound states ($E_1, E_2, \dots$). This trend is

especially prominent at low κ , where the impurity exerts minimal back-action on the condensate.

In contrast, κ primarily controls the feedback of the impurity onto the BEC. While it does not directly govern the number of impurity bound states, high values of κ can significantly modify the vortex structure and shift the effective trapping potential.

The white contour separating regions labeled 0 and 1 marks the localisation-delocalisation threshold for the impurity ground state: above this ridge at least one bound state is supported and below it the impurity remains delocalised.

These systematic trends corroborate the single case spectra presented in Figs. 6.4.2 and 6.4.1: the strong-coupling point ($\kappa=\nu=10$) lies deep inside the multi-bound state region, whereas $\kappa=1, \nu=1$ sits on the verge of delocalisation. This trend is consistent across vortex charges, as shown by the extended phase diagram for $s = 2$ and $s = 3$ in Fig. 6.4.6.

Comparison with related work:

In the bound state analysis of an impurity in a quantum vortex by Braz & Terças [7], the primary focus is on a regime where the condensate is weakly perturbed by the impurity, so that the BEC vortex effectively serves as a static background potential for the impurity. In contrast, our formulation introduces two dimensionless parameters:

$$\nu = \frac{m_i \chi_{2D}}{m g_{2D}} \quad \text{and} \quad \kappa = \frac{2 m \chi_{2D}}{\hbar^2},$$

We explore the regime where $\kappa \gtrsim 1, \nu \gtrsim 1$, beyond the weak-perturbation limit considered in Ref. [7]. By iteratively updating both the superfluid vortex and the impurity wave function, we capture strong back-action that yields additional and more deeply bound impurity levels, substantial vortex-core broadening, and parameter-dependent localisation thresholds.

In Ref. [17], the authors model the BEC by a fixed vortex profile (obtained from a Padé approximation), effectively treating the condensate as a static background potential for the impurity. This simplification enables them to calculate bound and excited impurity states in closed form and numerically, but it neglects the reciprocal effect of the impurity on the superfluid density. Our approach employs a fully coupled iterative scheme: we update both the superfluid vortex and the impurity wave-function, thereby capturing the back-action of the impurity on the vortex core. Consequently, we observe richer spatial modifications in the vortex density.

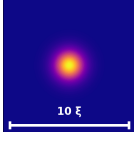
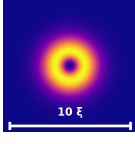
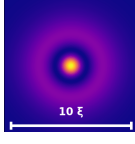
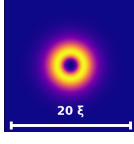
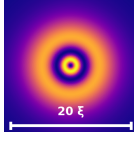
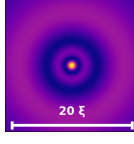
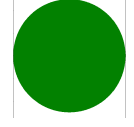
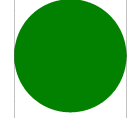
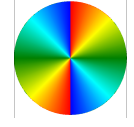
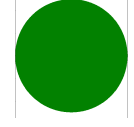
$ \phi'_{2D} $						
$\arg \phi'_{2D}$						
(n, ℓ)	(0,0)	(0,1)	(1,0)	(0,2)	(1,1)	(2,0)
E	2.056	3.667	4.494	4.768	4.908	4.969
ΔE	—	1.611	0.827	0.272	0.14	0.061

Table 6.1: **localised Impurity States for $\nu = 5$ and $\kappa = 1$.** The top rows show density plots of the impurity wave-functions $|g(r, \theta)|$ for selected radial and angular quantum numbers (n, ℓ) and corresponding phase. Energies are given E and the energy difference $\Delta E_n = E_n - E_{n-1}$, relative to the previous (lower) energy. As (n, ℓ) increase, the impurity wave-function exhibits additional radial or angular nodes, shifting the energy accordingly.

Table 6.1 collects the six impurity bound states that exist for the parameter set $\nu = 5$, $\kappa = 1$ and vortex charge $s = 1$. The ground state $(n, \ell) = (0, 0)$ is fully localised at the vortex axis with an isotropic density profile. Increasing either the radial quantum number n or the angular momentum ℓ introduces additional nodes and pushes probability weight towards larger radii, as seen in the density and phase plots. The energies E_n increase with the total number of nodes, while the spacing ΔE_n rapidly decreases from 1.61 to 0.06, reflecting the softer effective confinement at larger radii. This qualitative structure is similar to the spectrum obtained in [17], where the vortex profile is kept fixed; however, our fully coupled

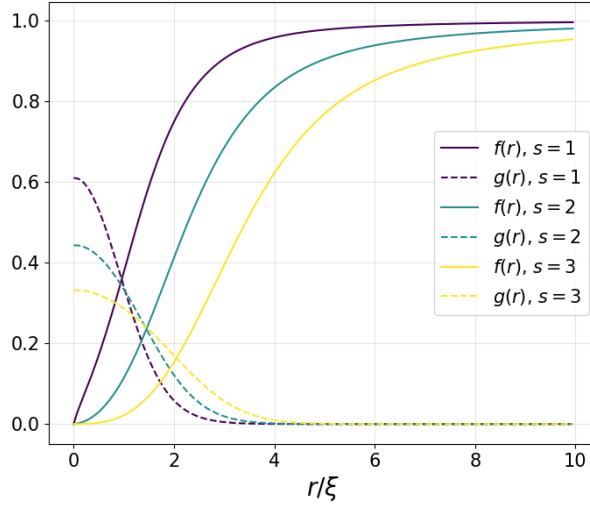
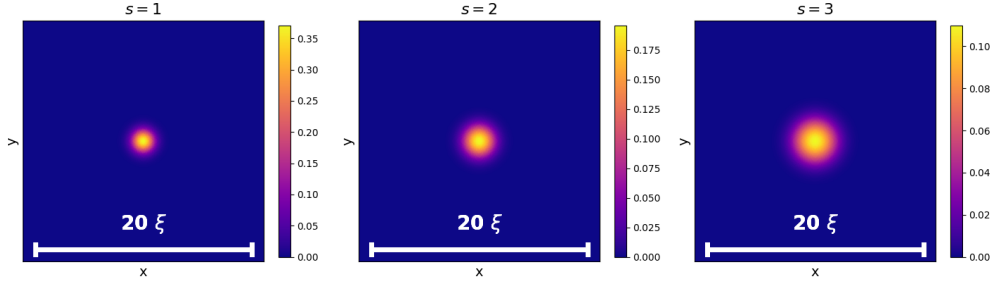
(a) Radial profiles $f(r)$ and $g(r)$ for $s = 1, 2, 3$ (b) 2D impurity density distributions for $s = 1, 2, 3$

Figure 6.4.4: (a) Radial superfluid background profiles $f(r)$ (solid lines) and impurity density profiles $g(r)$ (dashed lines) for vortex winding numbers $s = 1$, $s = 2$, and $s = 3$. (b) Corresponding 2D spatial distributions of the impurity density $|g(x, y)|^2$. As the vortex winding number increases, the superfluid core broadens and the impurity localisation adapts, spreading slightly but remaining centred within the vortex core.

calculation predicts slightly deeper low-lying levels and a modified spacing, due to the additional back-action of the impurity on the condensate density.

Although [17] mainly considers a singly quantised vortex ($s = 1$), our fully coupled iterative scheme extends to higher vortex winding numbers.

Higher vortex charge

The methodology extends to vortices with higher winding number $s > 1$. Figure 6.4.4 illustrates how the coupled condensate and impurity profiles change as s is increased from 1 to 3. Panel (a) shows the radial superfluid background $f(r)$ (solid lines) and impurity density profiles $g(r)$ (dashed lines) for $s = 1, 2, 3$ at fixed (κ, ν) . As s increases, the vortex core in $f(r)$ broadens and the impurity peak shifts slightly outward as the vortex core broadens, but the impurity density remains strongly localised within the core region. Panel (b) displays the corresponding two-dimensional impurity densities $|g(x, y)|^2$, confirming that localisation is always centred on the vortex axis, with a modest increase in the spatial extent as the core widens.

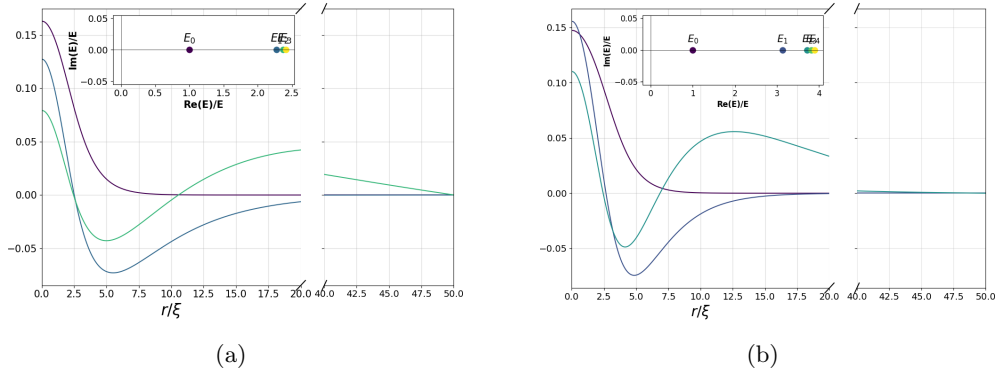


Figure 6.4.5: Impurity eigenstates and normalised eigenvalues for higher vortex winding numbers. (a) $s = 2$ case showing two localised impurity states; (b) $s = 3$ case showing three localised impurity states. Solid lines show the radial eigenfunctions $g(r)$; insets display the corresponding eigenvalues E_i in the complex plane. Increasing vortex winding number leads to larger vortex cores and a corresponding increase in the number of localised impurity states, consistent with the physical intuition that a broader superfluid depression can support more impurity modes.

For $s = 2$ Fig. 6.4.5(a) we find two localised impurity eigenstates, whereas for $s = 3$ Fig. 6.4.5(b) three bound states are supported. In each case the solid curves give the radial eigenfunctions $g_n(r)$, while the insets display the corresponding eigenvalues E_n . Increasing s leads to a broader and deeper effective density depletion, so that additional bound states can be supported at low energy. All eigenvalues are real within numerical precision.

Figure 6.4.6 (a) and (b) show the total number of localised impurity states as a function of (κ, ν) for $s = 2$ and $s = 3$, respectively. As in the $s = 1$ case, the number of bound states increases with both couplings and a distinct ridge separates regions with zero and one bound state, marking the localisation threshold for the impurity ground state. With increasing s this ridge shifts towards smaller values of κ and/or ν , reflecting the fact that a broader superfluid depression requires weaker couplings to trap the impurity. Overall, the higher-charge results confirm that our main conclusions for $s = 1$ core broadening, impurity localisation in the vortex core, and well-defined localisation-delocalisation boundaries in (κ, ν) space extend directly to multiquantum vortices.

6.5 Summary

We studied steady states of an impurity embedded in the core of a quantised vortex in a quasi-two-dimensional Bose–Einstein condensate. Using a self-consistent solution of the coupled Gross–Clark equations, we captured the impurity’s back-action on the condensate and obtained a richer impurity–vortex interaction than in static-vortex treatments.

Our results show that both the impurity-condensate coupling κ and the forward coupling ν control the number of bound impurity states, their spatial structure, and the deformation of the vortex core. The fully coupled approach reveals localisation-delocalisation transitions and the appearance of additional localised states driven by impurity-induced core modification. These findings show that a coupled description is required when modelling impurities in strongly interacting superfluids.

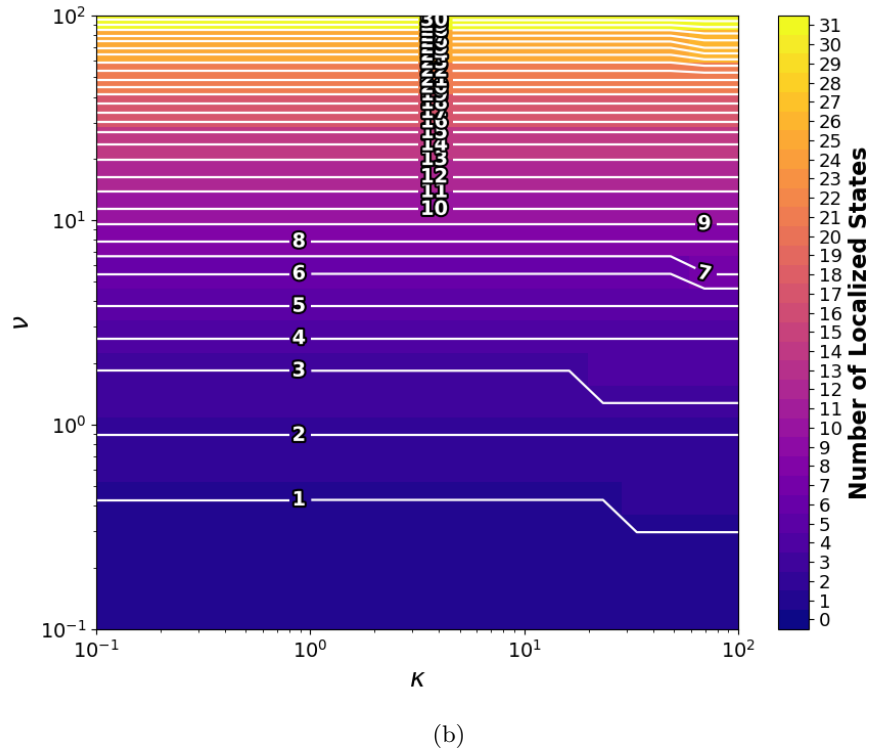
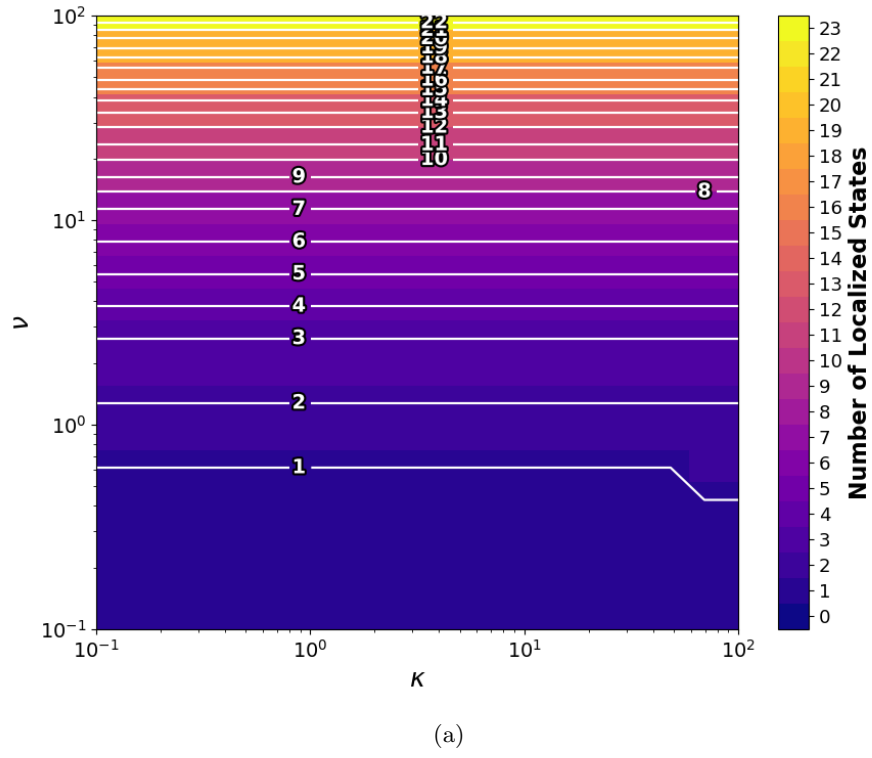


Figure 6.4.6: Number of localised impurity states as a function of interaction parameters κ and ν for vortex winding numbers (a) $s = 2$ and (b) $s = 3$. The colour map indicates the total number of bound impurity states supported by the superfluid background, with overlaid contours showing quantised levels. As with the $s = 1$ case, the number of localised states increases with both increasing ν and κ .

Dynamical vortex–impurity interactions

7.1 Overview and motivation

Quantised vortices are among the principal excitations of a trapped Bose–Einstein condensate (BEC). Their creation, stability, and interactions govern the dynamics of rotating condensates and are well described by the Gross–Pitaevskii and Bogoliubov frameworks [19]. While singly quantised vortices ($s = 1$) are dynamically stable solutions of the Gross–Pitaevskii equation in typical trapping geometries, multiply-charged vortices ($s > 1$) are energetically and dynamically unstable in confined geometries. In particular, linear stability analyses and experiments show that a doubly quantised vortex $s = 2$ supports an unstable quadrupole $m = 2$ Bogoliubov mode, which drives decay into two singly quantised vortices [42, 60, 29].

The primary objectives of this chapter are threefold. First, we examine impurity binding to a singly quantised vortex ($s = 1$), which is dynamically stable, in order to establish a baseline system and to investigate the decay and relaxation of impurity excited states in the absence of intrinsic vortex instabilities. Second, we characterise the dynamical splitting of a doubly quantised vortex ($s = 2$) in a finite bucket trap and analyse the subsequent undamped, recurrent two-vortex dynamics that arise following the decay of the $s = 2$ state in the clean

condensate. Third, we quantify how the presence of a localised impurity modifies the $s = 2$ dynamics, with particular emphasis on impurity-induced pinning, suppression of the unstable $m = 2$ Bogoliubov mode, and changes in the inter-vortex separation. By comparing impurity-free and impurity-coupled systems under identical numerical conditions, we assess whether a localised impurity can stabilise a doubly quantised vortex that would otherwise decay and quantify its influence on the ensuing vortex dynamics [19, 42, 60, 29, 44].

7.2 Model setup

7.2.1 Initial state and seeding

Stationary, axisymmetric vortex and impurity profiles are first constructed in polar coordinates (r, θ) . These radial solutions, obtained in Chapter 6, are then mapped to a two-dimensional Cartesian grid to initialise the real-time evolution.

Condensate. The stationary vortex profile $f(r)$ in the bucket trap $V(r)$ is obtained by relaxing the radial GPE using imaginary-time propagation as discussed in Chapter 6. In the dimensionless units used here the background chemical potential is normalised to one, giving the radial equation

$$f'' + \frac{1}{r}f' - \frac{s^2}{r^2}f + (1 - V(r))f - f^3 = 0, \quad (7.2.1)$$

The converged solution $f(r)$ is interpolated (cubic spline) onto a 2D Cartesian grid to initialise

$$\psi_0(r, \theta) = f(r)e^{is\theta}. \quad (7.2.2)$$

This provides the standard initial state of a singly or multiply quantised vortex in a finite bucket trap. Here ψ_0 denotes the initial condensate field, expressed in polar or Cartesian coordinates as appropriate.

Coupled condensate–impurity. With an impurity present, we solve the coupled Gross–Clark radial equations 6.1.2 in the same trap.

$$\begin{cases} f'' + \frac{1}{r}f' - \left(\frac{s^2}{r^2} + f^2 + \kappa g^2 - V - 1\right)f = 0, \\ g'' + \frac{1}{r}g' - \left(\frac{\ell^2}{r^2} + \nu f^2 - V\right)g = Eg, \end{cases}$$

The resulting radial solutions $f(r)$ and $g(r)$, obtained in Chapter 6 for a given vortex charge s and impurity angular momentum ℓ , are then mapped to a Cartesian grid to initialise the dynamics. V denotes the bucket trap, which confines both the condensate and the impurity in the finite domain.

$$\psi_0(x, y) = f(r)e^{is\theta}, \quad \phi_0(x, y) = g(r)e^{i\ell\theta},$$

with $r = \sqrt{x^2 + y^2}$ and $\theta = \arg(x + iy)$. These fields are then evolved in real time using the coupled Gross–Clark equations.

7.2.2 Bucket trap configuration (logistic wall)

Many trap shapes could be used to realise a finite bucket trap for the condensate, including harmonic traps and hard-wall potentials. Here we choose a circular box with a smooth logistic boundary, inspired by [44], which provides an effectively hard boundary without introducing numerical stiffness. A bucket trap provides a large, nearly uniform density region where vortex dynamics are not masked by strong density gradients, while still allowing confinement and recurrent dynamics.

Confinement is provided by a circular bucket trap described by the smooth logistic profile

$$V(r) = \frac{U_0}{1 + (U_0 - 1)e^{(r_B - r)/w}}, \quad (7.2.3)$$

which is essentially flat inside ($V \simeq 0$ for $r \ll r_B$) and tends to a high wall outside

($V \rightarrow U_0$). Throughout, we use

$$r_B = 25, \quad U_0 = 5, \quad w = \frac{1}{5}.$$

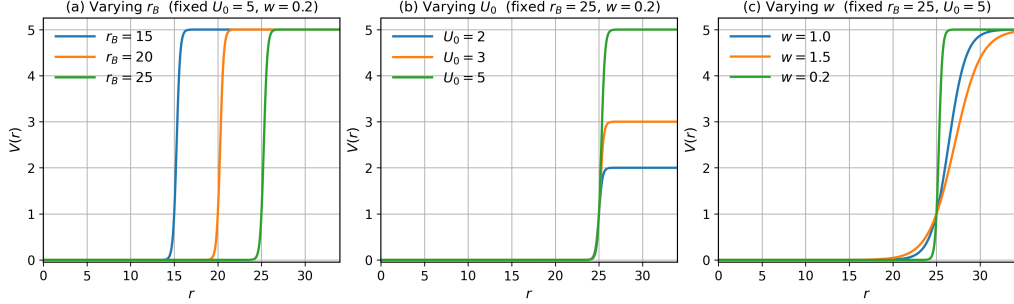


Figure 7.2.1: Logistic bucket trapping potential $V(r)$ defined in Eq. (7.2.3). (a) Effect of the bucket trap radius r_B at fixed wall height $U_0 = 5$ and wall width $w = 0.2$. (b) Effect of the wall height U_0 at fixed $r_B = 25$ and $w = 0.2$. (c) Effect of the wall width w at fixed $r_B = 25$ and $U_0 = 5$. In each case the potential is approximately flat inside the bucket trap and increases rapidly at the boundary, providing effective confinement.

The choice $r_B = 25$ gives a wide, nearly uniform cavity so that the vortex–core dynamics are well separated from the boundary. The value $U_0 = 5$ makes the density exponentially small beyond the wall, acting as an effective hard wall without introducing numerical stiffness, while $w = \frac{1}{5}$ produces a narrow but smooth edge, steep enough to confine the condensate.

The computational domain is chosen so that the low-density rim lies well inside the periodic boundaries, avoiding wrap-around artefacts as shown in Figure 7.2.2. This bucket trap configuration is standard for analysing vortex stability and splitting in trapped condensates [19, 44].

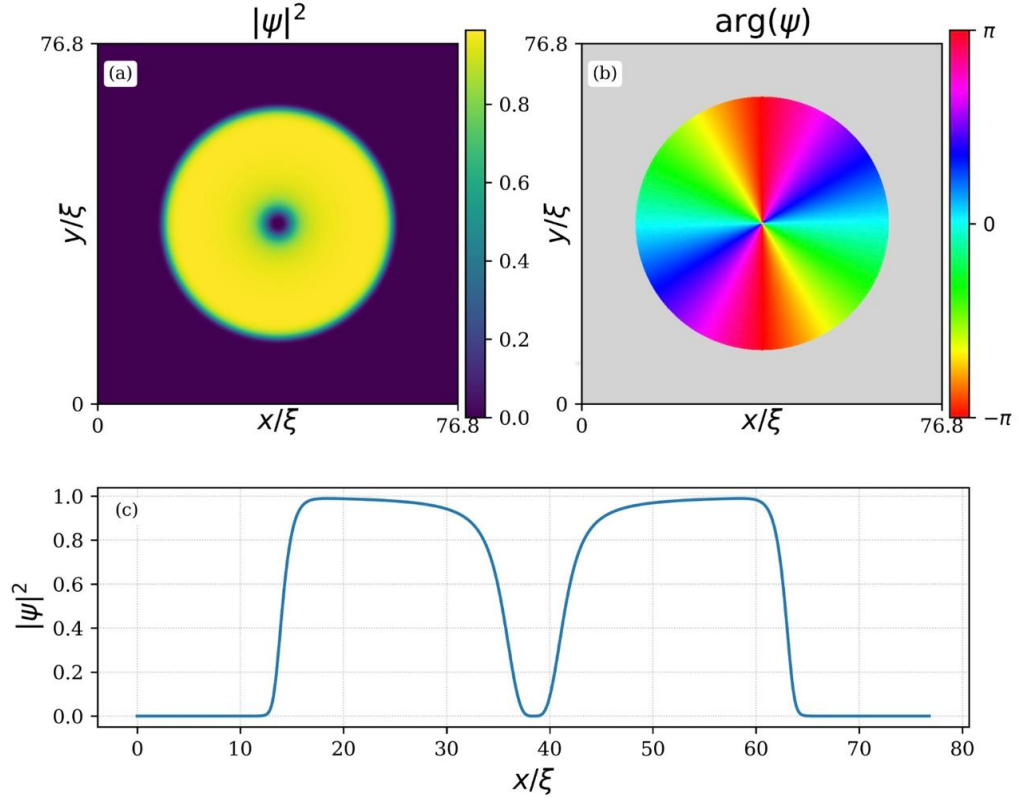


Figure 7.2.2: Stationary $s = 2$ vortex in the logistic bucket trap. (a) Condensate density $|\psi|^2$ on the full Cartesian grid, showing the central density dip and the flat bulk region inside the bucket trap. (b) Phase $\arg(\psi)$, with the 4π winding of the doubly quantised vortex visible around the origin. (c) Density profile $|\psi|^2$ along the horizontal centre line ($y = L/2$), illustrating the uniform interior, the vortex core at the centre, and the steep rise of the confining wall near the bucket trap radius.

7.2.3 Bogoliubov perturbation ($m = 2$)

Linearisation and azimuthal decomposition. We consider small excitations of the stationary vortex

$$\psi_0(r, \theta) = f(r)e^{is\theta} \quad (7.2.4)$$

in the same trap $V(r)$. The perturbation is added to the background vortex by expanding small deviations in azimuthal harmonics

$$\psi(r, \theta, t) = \psi_0(r, \theta) + \sum_{m \in \mathbb{Z}} \left[u_m(r)e^{im\theta - i\omega t} + v_m^*(r)e^{-im\theta + i\omega^* t} \right].$$

This decomposition exploits the axial symmetry of the stationary vortex, allowing different azimuthal sectors to decouple at the linear level.

Linearising the Gross–Pitaevskii equation in u_m and v_m gives, for fixed m , the radial Bogoliubov–de Gennes (BdG) system

$$\hat{L} \begin{pmatrix} u \\ v \end{pmatrix} = \omega \begin{pmatrix} u \\ v \end{pmatrix}, \quad \hat{L} = \begin{pmatrix} D_+ & \rho \\ -\rho & -D_- \end{pmatrix},$$

with

$$D_{\pm} = - \left(\partial_r^2 + \frac{1}{r} \partial_r - \frac{(s \pm m)^2}{r^2} \right) + V(r) + 2f^2(r) - 1. \quad (7.2.5)$$

The BdG system conserves the norm

$$N_{\text{BdG}} = \int (|u_m|^2 - |v_m|^2) d^2x, \quad (7.2.6)$$

and coupling between a positive–norm and a negative–norm branch produces a complex-conjugate pair of eigenvalues and thus a dynamical instability (the growing mode has $\text{Im} \omega > 0$). This mechanism underlies the $s = 2 \rightarrow 1 + 1$ decay in finite bucket traps and is absent in the large-trap limit where the branches decouple [19, 44].

Discretisation and boundaries. We discretise the BdG eigenproblem with $D_{\pm}$ given by Eq. (7.2.5) on a uniform radial grid using the same second-order finite-difference stencil for $\partial_r^2 + r^{-1} \partial_r$. Regularity at the origin is imposed by Robin conditions where $r_{\min}$ denotes the first nonzero radial grid point.

$$u'(r_{\min}) = \frac{s+m}{r_{\min}} u(r_{\min}), \quad v'(r_{\min}) = \frac{s-m}{r_{\min}} v(r_{\min}), \quad (7.2.7)$$

implemented in the first finite-difference row. At the outer boundary, where the condensate density is negligible, we set homogeneous Dirichlet data

$$u(r_{\max}) = v(r_{\max}) = 0. \quad (7.2.8)$$

This yields a $2N_I \times 2N_I$ matrix eigenproblem

$$AU = \omega U, \quad A = \begin{pmatrix} D_+ & F^2 \\ -F^2 & -D_- \end{pmatrix}, \quad (7.2.9)$$

where $D_{\pm}$ are the discrete single-particle blocks on the interior points and $F^2 = \text{diag}(f^2)$. We compute the spectrum with a dense eigensolver. Dense diagonalisation is used because the matrix dimension ($2N_I \lesssim 2000$) remains computationally manageable.

Mode used for seeding. The eigenpairs (ω_m, u_m, v_m) are ordered by growth rate $\text{Im} \omega_m$. For the $s = 2$ vortex, the most unstable excitation lies in the quadrupole sector $m = 2$. We therefore focus on the most unstable $m = 2$ mode $(u_m(r), v_m(r))$ and use it to seed the time-dependent simulations below. For visualisation we impose the normalisation

$$2\pi \int_0^{r_{\max}} (|u_m(r)|^2 + |v_m(r)|^2) r dr = 1, \quad (7.2.10)$$

while keeping track of the Bogoliubov norm defined in Eq. 7.2.6, whose sign labels each branch as having positive or negative norm. In the $s = 2$ case considered here, the unstable $m = 2$ mode originates from the coupling of a positive-norm and a negative-norm branch at an avoided crossing; the corresponding eigenvalue acquires a positive imaginary part $\text{Im} \omega > 0$ and drives the vortex-splitting dynamics. This unstable $m = 2$ mode provides the dominant dynamical channel through which the doubly quantised vortex decays in the time-dependent simulations discussed below.

Seeding the dynamics

We use the most unstable $m = 2$ Bogoliubov mode to initialise the real-time simulations, while no other unstable modes with $m \neq 2$ are present for $s = 2$ in this trap.

From the radial BdG calculation about ψ_0 we obtain the radial eigenfunctions $u_m(r)$ and $v_m(r)$ for $m = 2$ and build the corresponding small perturbation

$$\delta\psi(r, \theta) = \epsilon [u_m(r)e^{im\theta} + v_m^*(r)e^{-im\theta}], \quad m = 2, \quad (7.2.11)$$

with a fixed amplitude $\epsilon = 10^{-3}$. This perturbation has the angular dependence of the unstable BdG mode and is added only to the condensate field. The full initial condensate wavefunction is therefore

$$\psi(r, \theta, t = 0) = [f(r) + \delta\psi(r, \theta)]e^{is\theta}, \quad s = 2. \quad (7.2.12)$$

In all simulations the impurity field is initialised in its stationary state (Sec. 7.2.1) without any additional seed, so the vortex splitting is triggered solely by the condensate Bogoliubov mode. This procedure follows the standard preparation used in analyses of the doubly quantised vortex in the bucket trap [44, 45].

7.2.4 Time integration, boundary conditions, and diagnostics

We evolve the condensate and impurity fields ψ and ϕ in Cartesian coordinates on a 768×768 Fourier grid over a 76.8×76.8 domain with periodic boundary conditions. The corresponding spatial resolution $\Delta x = 0.1$ resolves the healing length by more than ten grid points, which is sufficient to capture the vortex-core structure and its deformation during splitting. Time stepping is performed using the same Strang split-step Fourier scheme described in Chapter 5, now applied in real time rather than imaginary time. The kinetic part is advanced in Fourier space, while the nonlinear and trapping contributions are applied in real space with timestep $\Delta t = 10^{-3}$. We also apply a standard 2/3 de-aliasing rule in Fourier space to remove spurious high-wavenumber components. [18, 2]. Convergence checks with finer grids (1024×1024) and smaller timesteps show no qualitative change in the dynamics, indicating numerical robustness.

All runs use the same trap, grid, timestep, and the same targeted $m = 2$ BdG

seed for the condensate, ensuring that differences between cases are due to the impurity. At each output we record conserved quantities (particle number N , linear momentum (P_x, P_y) , angular momentum L_z , and total energy E_{GC} to monitor conservation. Aliasing was checked explicitly by monitoring high-wavenumber spectral content, confirming that 2/3 de-aliasing removes spurious mode growth.

Vortex cores in the condensate are tracked using a pseudo-vorticity-based detector followed by Newton refinement and a circulation test along the lines of Villois’ Vortex Tracking Method ¹. Candidate points are identified as local maxima of a weighted pseudo-vorticity field

$$\omega_{\text{ps}} = \partial_x(\text{Re } \psi) \partial_y(\text{Im } \psi) - \partial_y(\text{Re } \psi) \partial_x(\text{Im } \psi),$$

with ω_{ps} computed from the spectral derivatives above and suppressed in high-density regions by a factor $(1 - \rho_\psi)^\beta$. Local maxima of this field above a given percentile threshold are taken as initial guesses. Each guess is refined by a Newton–Raphson iteration that uses the Jacobian of $(\text{Re } \psi, \text{Im } \psi)$, evaluated at the origin of a shifted coordinate patch, to converge to a phase zero. To avoid multiple detections of the same core we merge points closer than a fixed distance d_{min} .

For each refined core we then measure the circulation, Γ , by integrating the phase around a small circle of adaptive radius ϵ , chosen as a fraction of the inter-vortex separation but never smaller than a few grid spacings. Cores with $0.6 \leq |\Gamma| \leq 1.4$ are classified as singly quantised, where the tolerance accounts for numerical errors arising from discretisation and finite resolution; others are discarded as spurious. The minimal separation between any two such $|\Gamma| \approx 1$ cores is recorded as the inter-vortex distance $d(t)$, and vortex counts and $d(t)$ are stored as time series for subsequent analysis [65, 44].

¹See Ch. 3 of Villois’ thesis [64] for the Newton–Raphson refinement.

7.3 Results

7.3.1 Impurity bound to a singly quantised vortex ($s = 1$)

Core-localised impurity states ($\ell = 0, 1$)

Before analysing impurity effects on multiply quantised vortices, it is instructive to consider the simpler case of a singly quantised vortex ($s = 1$). In the absence of impurities, such a vortex is dynamically stable under Gross-Pitaevskii evolution and therefore provides a natural baseline for assessing impurity-vortex interactions.

We initialise the coupled system with a $s = 1$ vortex and place the impurity in a localised bound state obtained from the self-consistent radial problem in Chapter 6 for the interaction parameters $\kappa = 1$ and $\nu = 10$ chosen. Two cases are considered: the impurity ground state ($\ell = 0$) and a localised excited state ($\ell = 1$). The subsequent dynamics are analysed using real-time evolution of the coupled Gross-Clark equations.

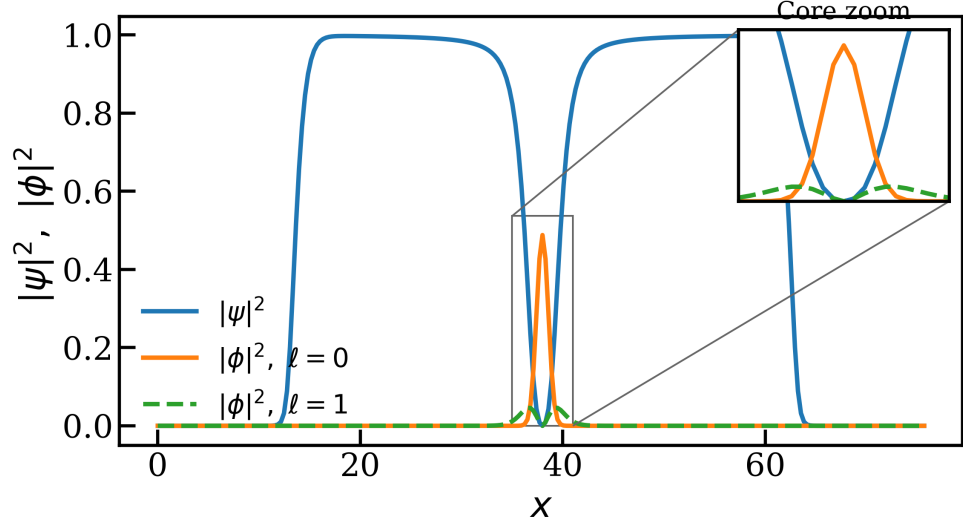
For the singly quantised vortex, no unstable Bogoliubov mode exists, and the system is therefore perturbed by adding a small random perturbation of amplitude 10^{-3} to the initial condensate wavefunction, in contrast to the targeted BdG seeding used in the $s = 2$ case.

To quantify the dynamical stability of impurity bound states, we introduce the overlap (or fidelity)

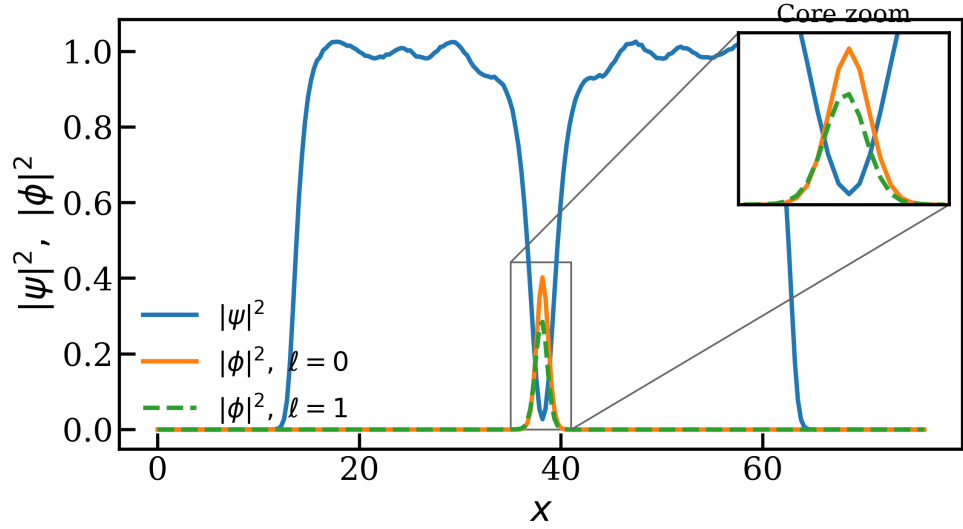
$$C_\ell(t) = \left| \int \phi_\ell^*(\mathbf{r}, 0) \phi(\mathbf{r}, t) d^2r \right|^2, \quad (7.3.1)$$

where $\phi_\ell(\mathbf{r}, 0)$ is the normalised impurity eigenstate used as the initial condition (with angular momentum ℓ), and $\phi(\mathbf{r}, t)$ is the impurity wavefunction at time t , normalised at each time step. The quantity $C_\ell(t) \in [0, 1]$ measures the similarity between the evolving impurity state and the initial eigenstate. Values close to unity indicate that the state remains dynamically stable, while a decay of $C_\ell(t)$

signals relaxation or decay away from the initial eigenstate.



(a)



(b)

Figure 7.3.1: One-dimensional density slices through the vortex centre for an $s = 1$ vortex with a bound impurity. (a) shows the initial profiles, demonstrating that both $\ell = 0$ (ground) and $\ell = 1$ (excited) impurity states are localised within the vortex core. At late times as shown in (b), the $\ell = 0$ impurity remains sharply localised, while the $\ell = 1$ impurity remains bound but exhibits reduced peak amplitude, consistent with relaxation to a lower-energy bound configuration.

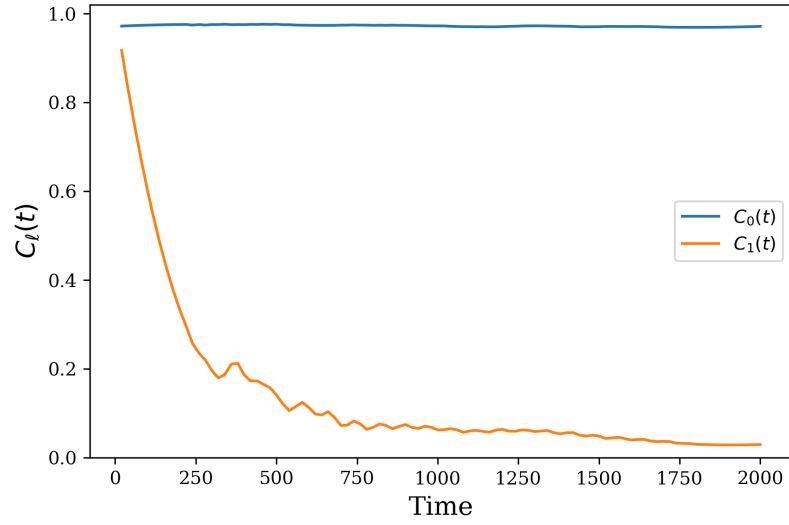


Figure 7.3.2: Time evolution of the overlap (fidelity) $C_\ell(t)$ between the impurity wavefunction and the initial impurity eigenstate for an impurity bound to an $s = 1$ vortex. The ground state impurity ($\ell = 0$) remains dynamically stable, with $C_0(t)$ staying close to unity throughout the evolution. In contrast, the excited impurity state ($\ell = 1$) exhibits a rapid decay of overlap, with $C_1(t)$ decreasing from near unity to a small value, indicating relaxation away from the initial excited eigenstate. Despite this decay, the impurity remains localised within the vortex core, as confirmed by density profiles.

Figure 7.3.1(a) shows one-dimensional density slices through the vortex centre for the initial configurations. Both the ground-state impurity ($\ell = 0$) and the excited impurity state ($\ell = 1$) are initially localised within the vortex core, with the impurity density confined to the central region of depleted condensate density. This confirms that both states correspond to vortex-bound impurity configurations at the level of the static problem.

The subsequent real-time dynamics are illustrated in Fig. 7.3.1(b). The ground-state impurity remains sharply localised at the vortex core, and the overall vortex structure is preserved throughout the evolution. In contrast, while the ($\ell = 1$) impurity relaxes to a lower-energy bound configuration while remaining trapped in the vortex core, consistent with energy transfer from the impurity to condensate excitations.

This behaviour is quantified in Fig. 7.3.2, which shows the time evolution of the

overlap (fidelity) between the impurity wavefunction and the initial impurity eigenstate. For the ground state ($\ell = 0$), the overlap remains close to unity, decreasing only weakly from $C_0 \simeq 0.97$ at early times to $C_0 \simeq 0.94$ over the simulated time window, demonstrating that the impurity ground state is dynamically stable when bound to an ($s = 1$) vortex. By contrast, the overlap for the excited state ($\ell = 1$) decays rapidly from near unity with $C_1(t)$ decreasing from $C_1 \simeq 0.98$ at $t = 10$ to $C_1 \simeq 0.02$ by $t \simeq 2000$, indicating relaxation away from the initial excited eigenstate.

Importantly, the decay of $(C_1(t))$ does not correspond to impurity delocalisation. As confirmed by the density profiles in Fig. 7.3.1(b), the impurity remains confined within the vortex core while relaxing to a lower-energy bound configuration. These results demonstrate that impurity binding alone does not destabilise a singly quantised vortex, but that excited impurity bound states are not dynamically robust under the full coupled evolution.

Overall, the ($s = 1$) vortex provides a clean reference case: the impurity ground state is dynamically stable, whereas excited impurity states relax through coupling to condensate excitations while remaining vortex-bound. This establishes a clear baseline for the more complex behaviour observed for multiply quantised vortices in the following sections.

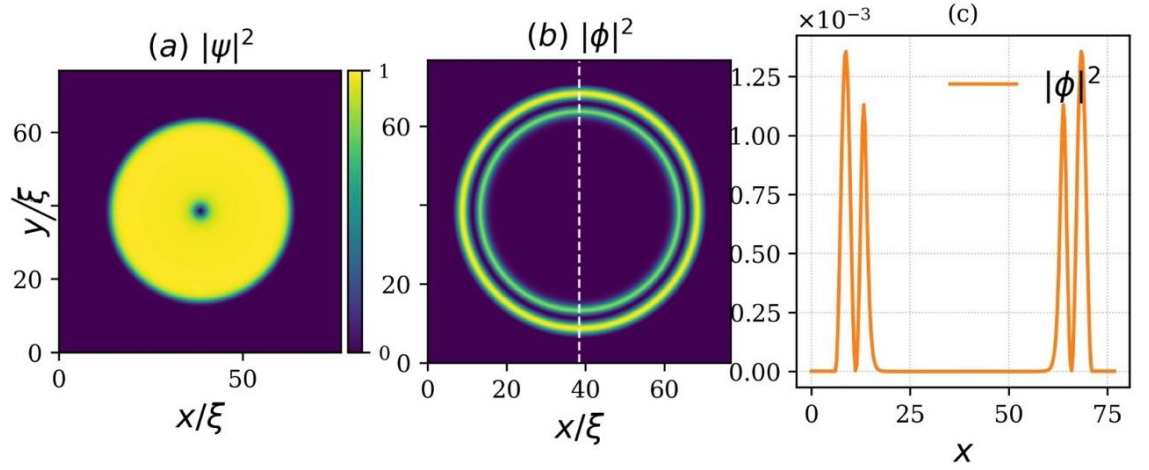


Figure 7.3.3: Impurity localisation at the edge of an $s = 1$ vortex for a second excited state with $\ell = 3$. (a) Condensate density $|\psi|^2$ showing a singly quantised vortex centred in the bucket trap. (b) Impurity density $|\phi|^2$ for the excited state $\ell = 3$, exhibiting a ring-shaped structure localised near the edge of the condensate rather than in the vortex core. The dashed line indicates the position of the one-dimensional slice. (c) Corresponding density slice $|\phi(x, y_0)|^2$, showing pronounced peaks close to the condensate boundary and negligible density at the vortex centre.

Edge-localised impurity states (higher ℓ)

In addition to core-localised impurity states, higher excited impurity modes can exhibit qualitatively different spatial localisation. Figure 7.3.3 shows the case of an impurity initialised in a higher angular momentum state ($\ell = 3$) in the presence of an $s = 1$ vortex. In this case the impurity density does not localise within the vortex core. Instead, $|\phi|^2$ forms a ring-like structure near the edge of the condensate, where the superfluid density rapidly decreases. The corresponding one-dimensional slice confirms that the impurity density is suppressed at the vortex centre and peaks close to the condensate boundary.

This behaviour can be understood as a consequence of the centrifugal barrier associated with higher angular momentum impurity states, which disfavors localisation at the vortex core and shifts the impurity towards regions of lower condensate density. The $\ell = 3$ state therefore represents an edge-localised impurity configuration rather than a vortex-bound state. This contrasts with

the $\ell = 0$ and $\ell = 1$ cases, where the impurity remains confined within the vortex core, and demonstrates that impurity localisation in an $s = 1$ vortex depends sensitively on the impurity angular momentum.

Having established this baseline behaviour for $s = 1$, we now turn to the more interesting case of a multiply quantised vortex, where impurity coupling can qualitatively modify an intrinsic dynamical instability.

7.3.2 Splitting dynamics of a doubly quantised vortex ($s = 2$)

Unlike the singly quantised vortex, a doubly quantised vortex ($s = 2$) is dynamically unstable and undergoes splitting even in the absence of an impurity.

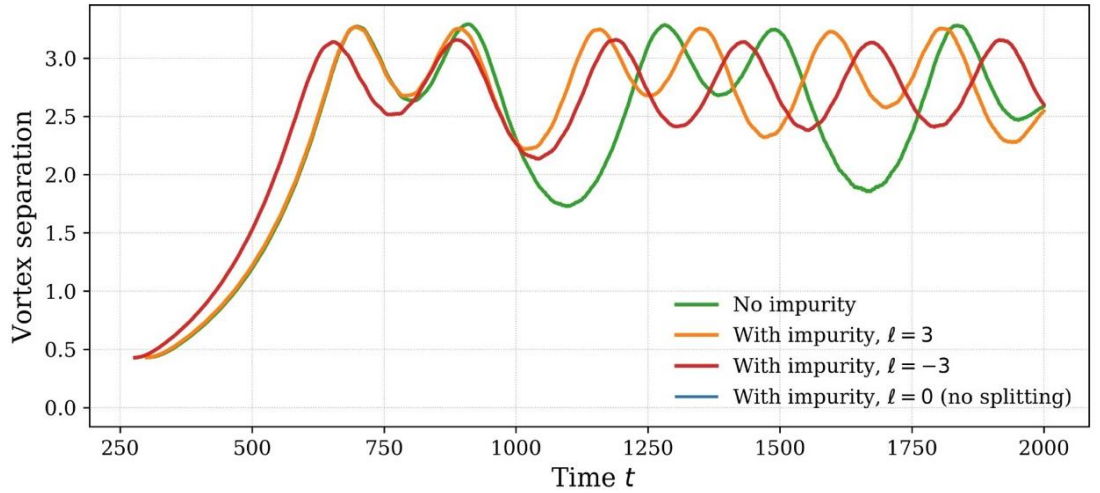


Figure 7.3.4: Vortex separation $d(t)$ for identical runs, including a clean condensate (no impurity) and selected impurity cases. All runs use the same trap, grid, timestep, and $m = 2$ BdG seed for the condensate. The clean BEC and the $\ell = \pm 3$ impurity cases split and show large-amplitude oscillations of $d(t)$, whereas for the $\ell = 0$ case no splitting is observed over the simulated time window.

Starting from the saved $s = 2$ state and adding a small $m = 2$ BdG seed ($\epsilon = 10^{-3}$), the vortex splits into two $s = 1$ vortices. Density and phase snapshots (Fig. 7.3.5) show the transition from a central 4π winding to two

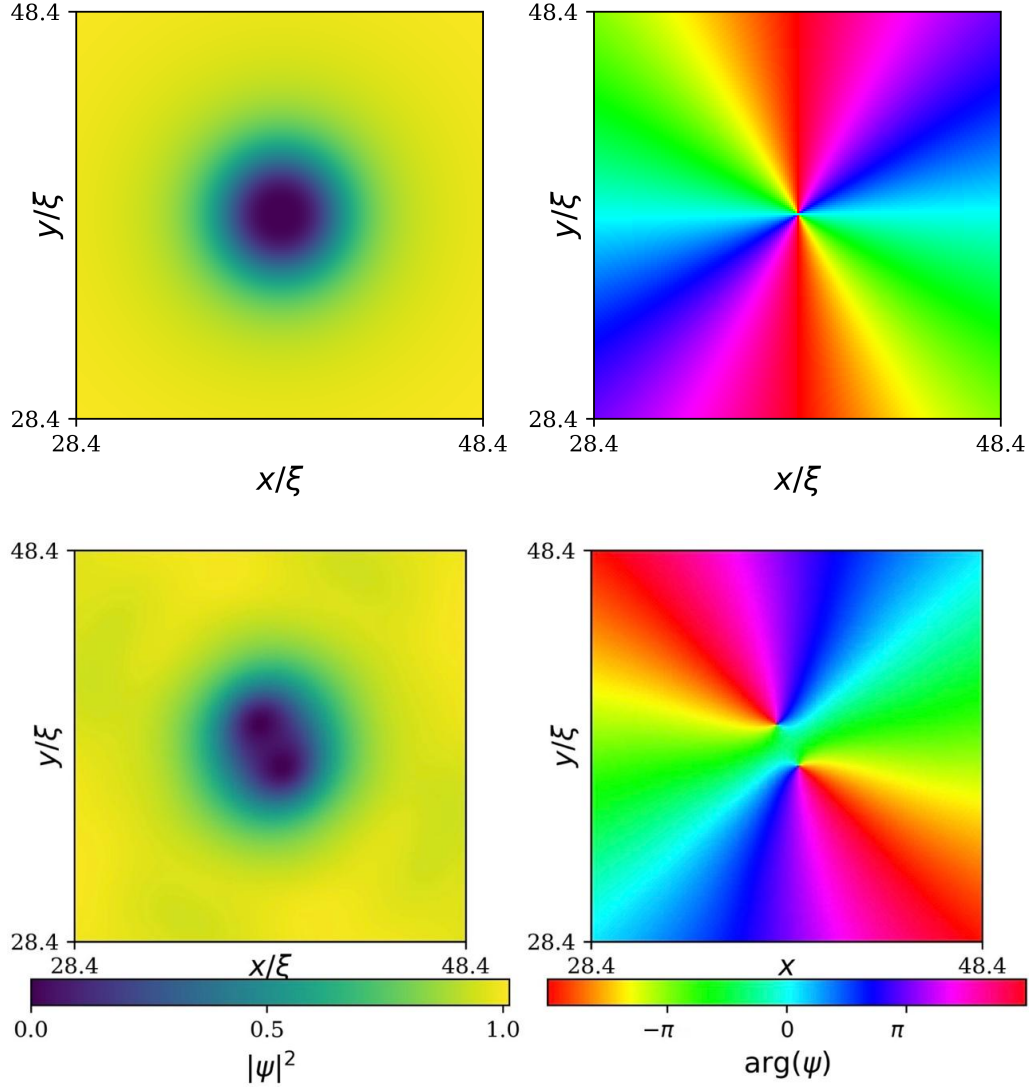


Figure 7.3.5: Density-phase snapshots for the condensate about the origin where the vortex is located. Left: density $|\psi|^2$. Right: phase $\arg \psi$. Top ($t = 0$): saved stationary $s = 2$ state with a single central density dip and 4π phase winding. Bottom ($t = 2000$): after adding the $m = 2$ BdG seed and evolving the GPE, the core splits into two $s = 1$ vortices.

separated 2π singularities while the net topological charge remains $+2$. The inter-vortex separation $d(t)$ grows rapidly from near zero and then enters a large-amplitude, quasi-periodic regime set by the trap. The pair remains confined in the bucket trap. This is the standard $m = 2$ dynamical instability of a doubly quantised vortex in finite traps.

Early-time growth and BdG consistency. From the radial BdG solve about the saved background, we obtain the most unstable mode with $\omega \approx 0.441447 + i 0.012665$ (residual 6.3×10^{-12} ; BdG norm $\approx 6.8 \times 10^{-5}$). The measured early-time growth rate, extracted from the linear window of $d(t)$, agrees with $\text{Im } \omega$ to within expected numerical tolerance, confirming that the seeded nonlinear run follows linear stability theory before saturation [19, 44].

Verification. Invariants (mass, linear momentum, angular momentum, and energy) drift negligibly at this resolution; halving the timestep and refining the grid do not change the qualitative outcome. Vortex cores are identified robustly by Newton refinement of phase zeros guided by pseudo-vorticity, with a circulation filter and a fixed merge threshold $d_{\min}$ to avoid duplicate detections [65].

7.3.3 Splitting dynamics of a doubly quantised vortex with an impurity

This subsection examines the dynamics of a doubly quantised vortex ($s = 2$) in a two-dimensional bucket trap in the presence of a localised impurity. We begin by incorporating a coupled impurity field ϕ localised at the vortex core. For the interaction parameters $\kappa = 1$ and $\nu = 10$ chosen in Chapter 6, the impurity supports several localised bound states labelled by the angular momentum quantum number ℓ . We focus on three representative cases: $\ell = 0$ and $\ell = \pm 3$. The $\ell = 0$ state is a localised, zero-angular-momentum impurity at the vortex core, while $\ell = \pm 3$ are the highest angular-momentum localised states that remain confined inside the $s = 2$ vortex.

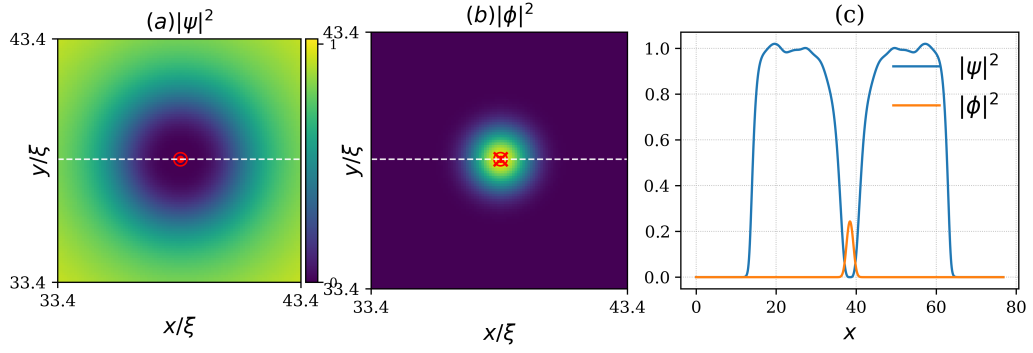


Figure 7.3.6: BEC-Impurity ($\ell = 0$) at late time ($t = 2000$). (a) Condensate density $|\psi|^2$; a single centred core is retained. (b) Impurity density $|\phi|^2$ remains localised near the vortex centre. (c) One-dimensional slice at $y = y_0$ (taken through the vortex centre) showing $|\psi|^2$ (blue) and $|\phi|^2$ (orange); the impurity peak sits inside the condensate density dip.

Core-localised impurity: stabilisation for $\ell = 0$ (zero-momentum impurity)

We initialise the condensate vortex from the stationary $s = 2$ state and superimpose a localised impurity with zero angular momentum ($\ell = 0$) centred on the vortex core. The impurity density $|\phi|^2$ is narrow compared with the core and sits where $|\psi|$ is minimal, so the two fields are co-located at $t = 0$. After adding the same targeted $m = 2$ BdG seed to the condensate field, we evolve with the same parameters, trap, grid and timestep. Over the entire simulation window the condensate does not split, and a single phase singularity (total charge $+2$) remains at the centre as in Fig. 7.3.6, and the measured inter-core separation stays below the vortex-tracking merge threshold $d_{\min}$ (Fig. 7.3.4). This behaviour is consistent with impurity-induced pinning that suppresses the $m = 2$ channel responsible for the $s = 2 \rightarrow 1+1$ decay in the impurity-free system. Physically, the impurity fills and deepens the vortex core, reducing its susceptibility to the quadrupole deformation [19, 44].

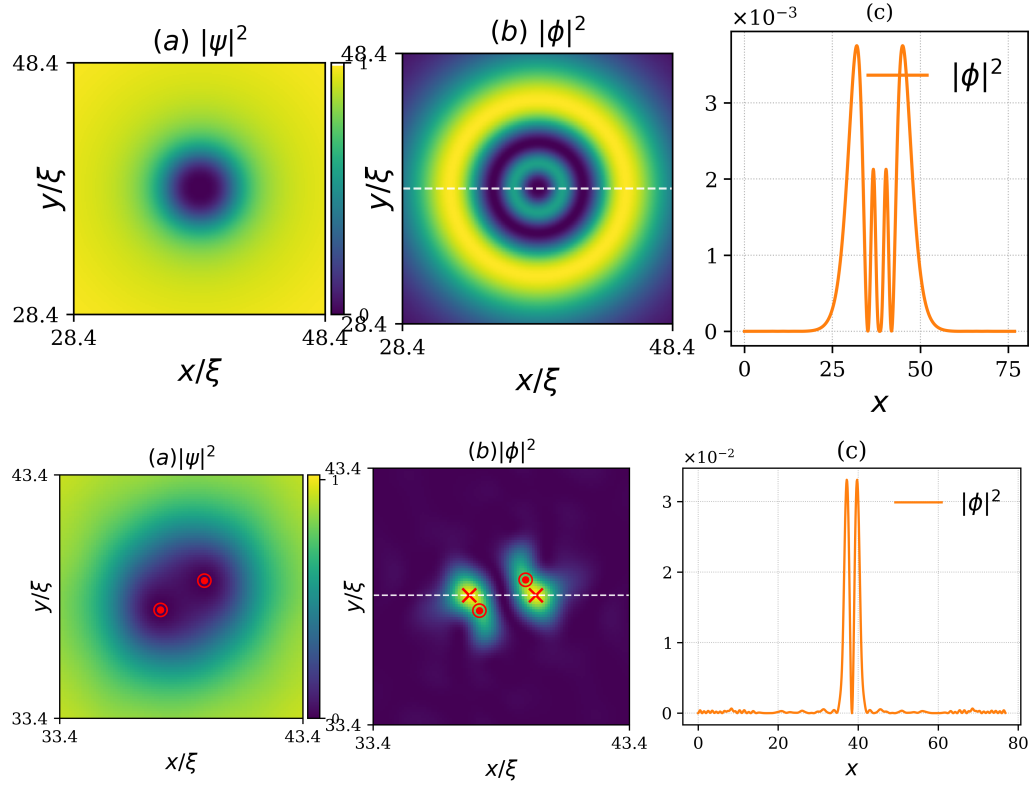


Figure 7.3.7: Co-rotating impurity case ($\ell = +3$). Top row ($t = 0$): initial fields—condensate density $|\psi|^2$ (left) and impurity density $|\phi|^2$ (middle) showing the multi-ring, multi-node $\ell = 3$ structure; right panel: one-dimensional slice of $|\phi|^2$ along the x -axis through the vortex centre. Bottom row ($t = 2000$): after evolution the condensate has split into two vortices and the impurity has relaxed from the excited $\ell = 3$ pattern into two narrow peaks. The right-hand slice is taken along the same axis, and the two impurity peaks lie close to the condensate vortex positions.

Co-rotating excited impurity: $\ell = +3$

We initialise the condensate vortex in the $s = 2$ state and place a localised impurity in the $\ell = +3$ eigenstate (a multi-node radial profile) centred on the vortex core. After applying the same $m = 2$ BdG seed to the condensate field, the condensate follows qualitatively the same splitting dynamics as in the condensate without impurity: the $s = 2$ core splits and a persistent two-vortex state forms. The inter-vortex separation curve (green in Fig. 7.3.4) crosses the detection threshold on the same time scale as the clean run and then oscillates with comparable amplitude and period, up to small phase and amplitude shifts.

Figure 7.3.7 shows that the impurity remains localised near the condensate vortices throughout the evolution but relaxes from its initial multi-node, $\ell = 3$ structure towards a single localised peak. One-dimensional slices of $|\phi|^2$ change from an oscillatory, multi-peak profile at $t=0$ to a single narrow peak by $t=2000$. In short, a co-rotating excited impurity survives the splitting process but quickly sheds its $\ell=3$ character and behaves as a weak spectator. The condensate dynamics remain close to the impurity-free case with a slightly smaller amplitude.

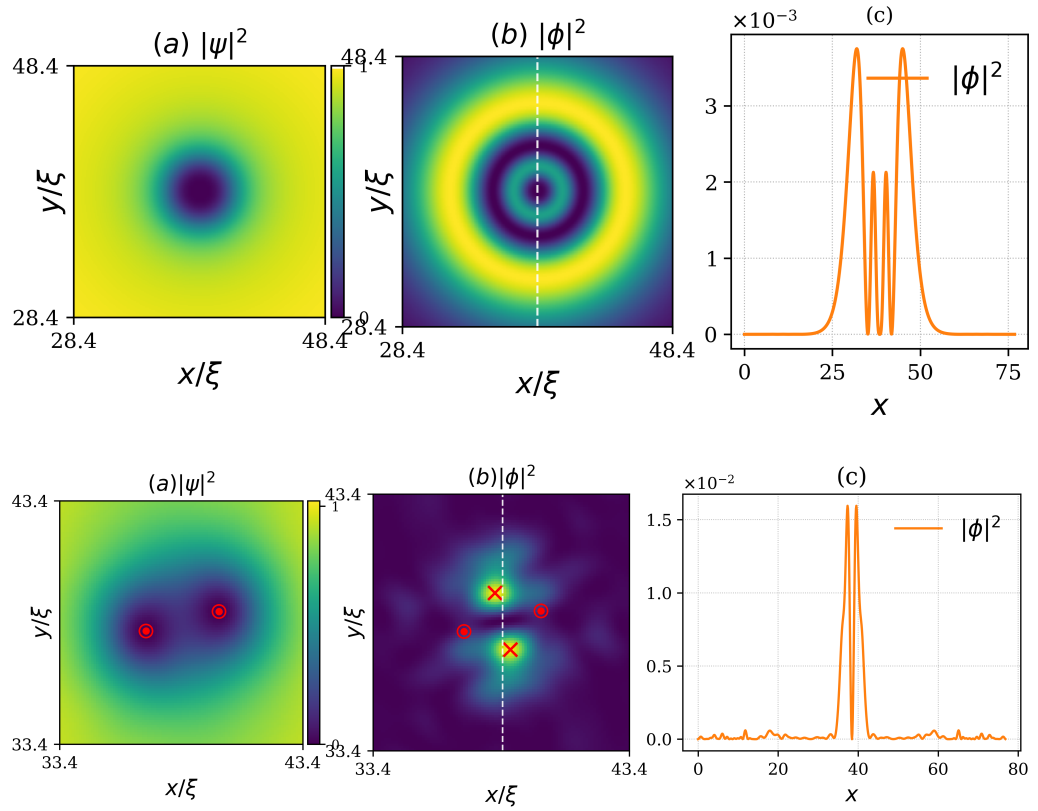


Figure 7.3.8: Counter-rotating impurity case ($\ell = -3$). Top row ($t = 0$): condensate density $|\psi|^2$ (left) and impurity density $|\phi|^2$ (middle) with a localised, multi-ring profile; right panel: one-dimensional slice of $|\phi|^2$ along the x -axis through the vortex centre. Bottom row ($t = 2000$): the condensate has split into two $s = 1$ vortices, while the impurity has relaxed into a multi-peak state concentrated near, but not exactly on, the vortex pair (right: 1D slice), indicating loss of the initial ring structure and partial off-core localisation.

Counter-rotating excited impurity: $\ell = -3$

We initialise the condensate vortex in the $s = 2$ state and place a localised impurity in the counter-rotating $\ell = -3$ eigenstate (a multi-node density near the core at $t = 0$). After seeding the $m = 2$ mode and evolving, the condensate vortex follows qualitatively the same splitting process observed in the condensate run: the $s = 2$ core splits and a persistent two-vortex state forms. The inter-vortex separation signal (red curve in Fig. 7.3.4) grows and then oscillates with a period and amplitude comparable to the clean run.

The impurity response is different from the co-rotating case. Figure 7.3.8 shows that the impurity no longer remains on the vortex cores. Instead, $|\phi|^2$ develops off-core maxima located near, but not coincident with, the vortex positions. The slice of $|\phi|^2$ changes from a multi-peak profile at $t = 0$ to a single narrow peak that is displaced from the cores. Thus a counter-rotating excited impurity is repelled from the vortex centres and redistributes into nearby off-core lobes. This behaviour is consistent with the effective centrifugal barrier for counter-rotating modes, which disfavors binding exactly at the vortex centre. The condensate dynamics remain broadly similar to those in the impurity-free run.

Overall, excited $\ell = \pm 3$ impurities do not suppress the $m = 2$ driven splitting; they relax away from their initial angular content and provide at most a weak perturbation to the post-split vortex motion.

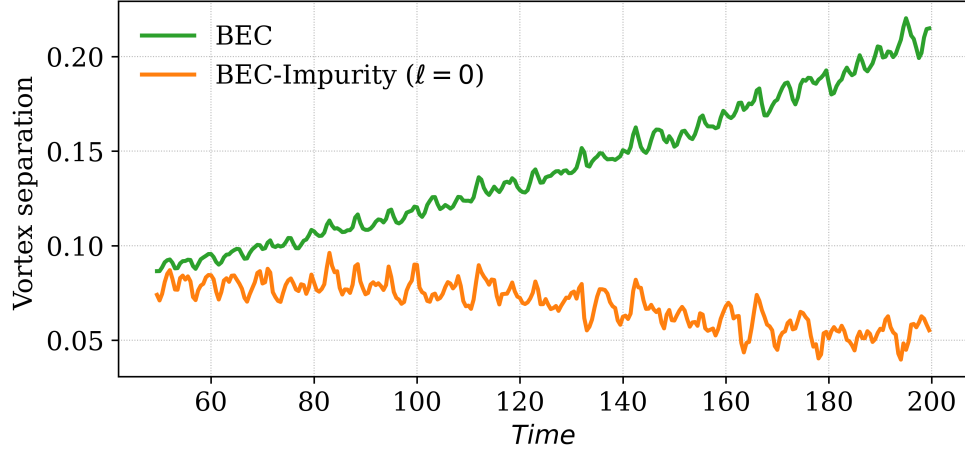


Figure 7.3.9: Inter-vortex separation $d(t)$ for the clean condensate (green) and the run with a localised $\ell = 0$ impurity (orange). Both runs use the same trap, grid, timestep, and $m = 2$ seed. The clean case shows splitting and large-amplitude oscillations of $d(t)$, whereas with the impurity present $d(t)$ remains small and slowly decays.

7.3.4 Main findings

Under identical numerics (trap, grid, timestep, $m=2$ BdG seed and tracker), a localised impurity in the $\ell=0$ state prevents the splitting of a doubly quantised vortex. No two-core state is detected across the full window above a threshold distance, even when the tracking merge threshold is tightened well below the default ($d_{\min} \ll 0.01$) and for long integrations ($t \leq 2 \times 10^4$). By contrast, in the clean $s = 2$ condensate the core splits, and the inter-core distance enters the well-known large-amplitude, quasi-periodic regime for bucket traps, in line with BdG/GPE expectations for the $m=2$ instability.

Figure 7.3.9 compares the early-time inter-vortex separation for the clean condensate and the run with a localised impurity ($\ell = 0$). In the clean case the separation grows steadily over $t \in [50, 200]$, reaching ≈ 0.21 , consistent with the onset of the $m = 2$ splitting. With the impurity present the separation remains bounded in the range 0.04–0.09, well within the detection threshold for split-core identification, and shows a weak downward trend, indicating that no

split develops under identical seeding and numerics.

The comparison implies that a centred impurity modifies the core so as to pin and suppress the unstable $m = 2$ mode in a doubly quantised vortex [19, 44].

7.4 Summary

This chapter first examined impurity binding to a singly quantised vortex ($s = 1$), which is dynamically stable, in order to establish a baseline system and to assess the decay and relaxation of impurity excited states in the absence of intrinsic vortex instabilities. We then investigated the $s = 2$ vortex in a trapped condensate, comparing the clean case with impurity-coupled systems under identical numerics and an $m = 2$ BdG seed. In the condensate without impurity the core splits into two $s = 1$ vortices and the separation oscillates, consistent with established analyses of the $m = 2$ instability in bucket traps. A localised $\ell = 0$ impurity prevents splitting throughout long runs ($t \leq 2 \times 10^4$) and for relaxed merge thresholds ($d_{\min} = 0.01 \rightarrow 0.4$), indicating pinning and suppression of the unstable $m = 2$ channel. Excited impurities with $\ell = \pm 3$ relax away from their initial angular structure and do not stabilise the vortex core. Hence a robust, centred impurity can stabilise a doubly quantised vortex that otherwise undergoes $s = 2 \rightarrow 1 + 1$ splitting.

Part III

Conclusions and Future Work

Conclusions

8.1 Conclusions

This thesis has investigated the behaviour of a quantum impurity embedded in a quasi-two-dimensional Bose-Einstein condensate, with particular emphasis on impurity self-localisation and impurity-vortex interactions. The analysis was carried out within the Gross-Pitaevskii and Gross-Clark frameworks, combining analytical arguments with systematic numerical simulations.

The theoretical foundations were established by deriving and analysing the Gross-Pitaevskii equation in dimensionless form and in the quasi-two-dimensional limit, with particular attention to the structure and properties of quantised vortices. This provided the background condensate states against which impurity effects were studied. To build physical intuition for impurity confinement, the linear Schrödinger equation was then analysed in one and two dimensions for a range of idealised trapping potentials, clarifying the distinction between localised and delocalised states.

The coupled condensate-impurity problem was formulated using the Gross-Clark model, reduced to an effective two-dimensional description and expressed in terms of a small set of dimensionless parameters. Numerical methods based on spectral discretisation and split-step time integration were developed and validated through extensive convergence and conservation checks.

Using this framework, the thesis first demonstrated that a single impurity can self-localise in an otherwise homogeneous condensate due to nonlinear feedback between the impurity and the condensate density. A variational analysis provided an estimate of the localisation threshold, which was confirmed and refined by direct numerical simulations. Allowing for asymmetric impurity-condensate couplings extended previous symmetric models and revealed a broader and more flexible localisation phase diagram.

The study was then extended to impurities trapped in the cores of quantised vortices. The vortex-induced density depletion was shown to act as an effective trapping potential supporting impurity bound states. The number and structure of these states were characterised as functions of the coupling parameters and vortex charge, and the role of impurity back-action on the vortex profile was quantified. Robust numerical criteria were developed to distinguish localised from delocalised impurity states on finite computational domains.

Finally, the thesis examined the dynamical consequences of impurity-vortex coupling. Real-time simulations demonstrated that a localised impurity can significantly modify vortex dynamics, including suppressing the splitting instability of a multiply quantised vortex. These results show that impurities can qualitatively alter the stability and dynamics of topological excitations in quantum fluids.

Overall, this work provides a coherent and systematic account of impurity localisation and impurity-vortex interactions in two-dimensional quantum fluids within a mean-field description. The results establish a foundation for future studies extending to finite temperatures, three-dimensional geometries, and systems with multiple interacting impurities, where additional physical effects beyond mean-field theory are expected to play an important role.

8.2 Future Work

The work presented in this thesis can be extended in several directions.

A first extension would be to include finite-temperature effects. The present study is restricted to zero-temperature mean-field dynamics, whereas thermal fluctuations are known to influence impurity motion, damping, and vortex stability. Incorporating finite-temperature models, such as dissipative or stochastic Gross-Pitaevskii approaches, would allow a more direct comparison with experiments.

A second direction concerns extensions beyond mean-field theory. While the Gross-Clark model captures the leading-order condensate deformation induced by an impurity, it neglects quantum fluctuations and correlation effects. Including beyond-mean-field corrections would enable a closer connection to polaron physics and clarify the limits of validity of the mean-field description.

The present work focuses on quasi-two-dimensional geometries. Extending the analysis to fully three-dimensional systems would allow the study of impurity interactions with vortex lines, vortex rings, and reconnection events, and would be relevant for a broader class of experimental configurations.

Another natural extension is the study of multiple impurities. Interactions mediated by the condensate could lead to collective effects such as clustering, effective impurity-impurity forces, or impurity-induced modifications of vortex lattices. This would provide insight into many-body impurity physics in quantum fluids.

Finally, further work could explore driven and non-equilibrium scenarios, such as externally forced impurities or time-dependent trapping potentials. These situations may give rise to new dynamical regimes and provide additional mechanisms for controlling vortex behaviour through impurity coupling.

Part IV

APPENDICES

A

Derivations for the Gross-Clark Model

A.1 Calculation of the Two-Dimensional Interaction Parameters χ_{2D} and g_{2D}

The Two-Dimensional Interaction Parameter χ_{2D}

The Gaussian wave-functions of the ground state for particles of masses m and m_i confined in a harmonic potential with frequency w are given by:

$$\psi_{\text{conf}}(z) = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega_z z^2}{2\hbar}}, \quad \phi_{\text{conf}}(z) = \left(\frac{m_i\omega_{z,i}}{\pi\hbar}\right)^{1/4} e^{-\frac{m_i\omega_{z,i} z^2}{2\hbar}}$$

The probability densities, or the squared magnitudes of these wave-functions, are:

$$|\psi_{\text{conf}}(z)|^2 = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega_z z^2}{\hbar}}, \quad |\phi_{\text{conf}}(z)|^2 = \left(\frac{m_i\omega_{z,i}}{\pi\hbar}\right)^{1/2} e^{-\frac{m_i\omega_{z,i} z^2}{\hbar}}$$

The integral of their product of these densities, crucial for the interaction term, is calculated as follows:

$$\int |\psi_{\text{conf}}(z)|^2 |\phi_{\text{conf}}(z)|^2 dz = \left(\frac{m\omega_z}{\pi\hbar}\right)^{1/2} \left(\frac{m_i\omega_{z,i}}{\pi\hbar}\right)^{1/2} \int e^{-\frac{(m\omega_z + m_i\omega_{z,i})z^2}{\hbar}} dz$$

Using the standard Gaussian integral formula ($\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$), the integral over all z is:

$$\int_{-\infty}^{\infty} e^{-\frac{(m\omega_z + m_i\omega_{z,i})z^2}{\hbar}} dz = \sqrt{\frac{\pi\hbar}{(m\omega_z + m_i\omega_{z,i})}}$$

This results in:

$$\int |\psi_{\text{conf}}(z)|^2 |\phi_{\text{conf}}(z)|^2 dz = \frac{\sqrt{(m\omega_z m_i\omega_{z,i})}}{\pi\hbar} \sqrt{\frac{\pi\hbar}{(m\omega_z + m_i\omega_{z,i})}} = \sqrt{\frac{(m\omega_z m_i\omega_{z,i})}{\pi\hbar(m\omega_z + m_i\omega_{z,i})}}$$

Combining these results, the effective two-dimensional interaction parameter χ_{2D} is derived as:

$$\chi_{2D} = \chi \sqrt{\frac{m\omega_z m_i\omega_{z,i}}{\pi\hbar(m\omega_z + m_i\omega_{z,i})}} = \frac{\chi}{\sqrt{\pi(a_z^2 + a_i^2)}}$$

where the characteristic lengths of the harmonic oscillator for each species are:

$$a_z = \sqrt{\frac{\hbar}{m\omega}}, \quad a_i = \sqrt{\frac{\hbar}{m_i\omega_{z,i}}}$$

The Two-Dimensional Interaction Parameter g_{2D}

$$g_{2D} = g \int |\psi_{\text{confined}}(z)|^4 dz$$

Using the standard Gaussian integral formula ($\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$), the integral required for the interaction term is:

$$\int |\psi_{\text{conf}}(z)|^4 dz = \left(\frac{m\omega_z}{\pi\hbar}\right) \int e^{-\frac{2m\omega_z z^2}{\hbar}} dz = \sqrt{\frac{m\omega_z}{2\pi\hbar}}$$

So the effective two-dimensional interaction strength is thus calculated as:

$$g_{2D} = \frac{g}{a_z \sqrt{2\pi}}$$

where a_z is the characteristic length of the oscillator, $a_z = \sqrt{\frac{\hbar}{m\omega_z}}$

A.2 Three-Dimensional Dimensionless Gross-Clark Equations

We start from the three-dimensional Gross-Clark (GC) system

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (g|\psi|^2 + \chi|\phi|^2) \psi, \quad (\text{A.2.1a})$$

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla^2 \phi + \chi|\psi|^2 \phi, \quad (\text{A.2.1b})$$

which couple the BEC order parameter $\psi(\mathbf{r}, t)$ (mass m) to an impurity field $\phi(\mathbf{r}, t)$ (mass m_i). The boson-boson and boson-impurity couplings are g and χ , respectively. In an untrapped three-dimensional condensate of bulk density ρ_{3D} , the chemical potential is $\mu = g\rho_{3D}$. The length scale is defined as $\xi = \sqrt{\frac{\hbar^2}{2m\mu}}$ and the time scale is derived from the speed of sound: $c = \sqrt{\mu/m}$. The wavefunctions ψ and ϕ are scaled as follows:

$$\psi \rightarrow \sqrt{\rho_{3D}} \tilde{\psi} e^{-i\mu t/\hbar}, \quad \phi \rightarrow \frac{\tilde{\phi}}{\xi^{3/2}},$$

where $\tilde{\psi}$ and $\tilde{\phi}$ are dimensionless. Substituting these definitions into (A.2.1a) and simplifying:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} [\sqrt{\rho_{3D}} \tilde{\psi} e^{-i\mu t/\hbar}] &= -\frac{\hbar^2}{2m} \nabla^2 [\sqrt{\rho_{3D}} \tilde{\psi} e^{-i\mu t/\hbar}] + g\rho_{3D} |\tilde{\psi}|^2 \sqrt{\rho_{3D}} \tilde{\psi} e^{-i\mu t/\hbar} \\ &\quad + \chi \frac{|\tilde{\phi}|^2}{\xi^3} \sqrt{\rho_{3D}} \tilde{\psi} e^{-i\mu t/\hbar}. \end{aligned}$$

Using $g\rho_{3D} = \mu$ and $\hbar^2/(2m\xi^2) = \mu$, dividing by μ and $e^{-i\mu t/\hbar}$, and switching to dimensionless variables yields

$$i \frac{\partial \tilde{\psi}}{\partial t} = -\nabla'^2 \tilde{\psi} + |\tilde{\psi}|^2 \tilde{\psi} + \kappa |\tilde{\phi}|^2 \tilde{\psi} - \tilde{\psi}, \quad (\text{A.2.2})$$

Applying the same rescaling to (A.2.1b), substituting $\phi = \tilde{\phi}/\xi^{3/2}$:

$$i\hbar \frac{\partial}{\partial t} \left(\frac{\tilde{\phi}}{\xi^{3/2}} \right) = -\frac{\hbar^2}{2m_i} \nabla^2 \left(\frac{\tilde{\phi}}{\xi^{3/2}} \right) + \chi |\sqrt{\rho_{3D}} \tilde{\psi}|^2 \frac{\tilde{\phi}}{\xi^{3/2}}.$$

Using $\xi^2 = \frac{\hbar^2}{2m\mu}$ and multiplying by $\xi^{3/2}/\mu$ obtain:

$$i\tau \frac{\partial \tilde{\phi}}{\partial t} = -\nabla'^2 \tilde{\phi} + \nu |\tilde{\psi}|^2 \tilde{\phi}, \quad (\text{A.2.3})$$

The fully dimensionless three-dimensional Gross-Clark equations are therefore

$$i \partial_{t'} \tilde{\psi} = -\nabla'^2 \tilde{\psi} + |\tilde{\psi}|^2 \tilde{\psi} + \kappa |\tilde{\phi}|^2 \tilde{\psi} - \tilde{\psi}, \quad (\text{A.2.4a})$$

$$i \tau \partial_{t'} \tilde{\phi} = -\nabla'^2 \tilde{\phi} + \nu |\tilde{\psi}|^2 \tilde{\phi}, \quad (\text{A.2.4b})$$

which depend only on the dimensionless parameters

$$\tau = \frac{m_i}{m}, \quad \kappa = \frac{\chi}{\mu \xi^3}, \quad \nu = \frac{m_i \chi}{mg}.$$

Equations (A.2.4) constitute the starting three-dimensional studies reported in this work.

A.3 Two-Dimensional Dimensionless Gross-Clark Equations

We consider a coupled BEC–impurity system described by:

$$\begin{aligned} i\hbar \frac{\partial \psi_{2D}}{\partial t} &= -\frac{\hbar^2}{2m} \nabla_{2D}^2 \psi_{2D} + \left(g_{2D} |\psi_{2D}|^2 + \chi_{2D} |\phi_{2D}|^2 \right) \psi_{2D} - \mu_{2D} \psi_{2D}, \\ i\hbar \frac{\partial \phi_{2D}}{\partial t} &= -\frac{\hbar^2}{2m_i} \nabla_{2D}^2 \phi_{2D} + \chi_{2D} |\psi_{2D}|^2 \phi_{2D} - E_{2D} \phi_{2D}. \end{aligned}$$

We now introduce dimensionless variables to simplify the analysis. We assume the

Bose–Einstein condensate (BEC) extends infinitely while the impurity remains localised. In the bulk (far from the impurity), the system of equations admits the solution

$$\begin{aligned}\psi_{2D}(\text{bulk}) &\rightarrow \sqrt{\rho} e^{-i \frac{\mu t}{\hbar}}, \quad \text{where} \quad \mu = g \rho + \mu_{2D}, \\ |\phi|(\text{bulk}) &\rightarrow 0,\end{aligned}$$

where ρ is the two-dimensional (surface) density of the bosons.

From this, we define two key physical quantities: The healing length,

$$\xi = \sqrt{\frac{\hbar^2}{2m\mu}},$$

The speed of sound,

$$c = \sqrt{\frac{\mu}{m}}.$$

To proceed with the dimensionless formulation, we scale the coordinates (x, y) by the healing length:

$$x' = \frac{x}{\xi}, \quad y' = \frac{y}{\xi},$$

and we rescale time by

$$t' = \frac{t c}{\sqrt{2} \xi}.$$

For the BEC wave-function ψ_{2D} , we divide by $\sqrt{\rho}$ (the square root of the boson surface density), while for the impurity ϕ_{2D} we divide by ξ . Thus:

$$\psi'_{2D} = \frac{\psi_{2D}}{\sqrt{\rho}}, \quad \phi'_{2D} = \frac{\phi_{2D}}{\xi}.$$

Starting with $\psi_{2D} = \sqrt{\rho} \psi'_{2D}$:

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} (\sqrt{\rho} \psi'_{2D}) &= -\frac{\hbar^2}{2m} \nabla_{2D}^2 (\sqrt{\rho} \psi'_{2D}) \\
&+ g_{2D} \rho |\psi'_{2D}|^2 \sqrt{\rho} \psi'_{2D} \\
&+ \chi_{2D} \xi^2 |\phi'_{2D}|^2 \sqrt{\rho} \psi'_{2D} \\
&- \mu_{2D} \sqrt{\rho} \psi'_{2D}.
\end{aligned} \tag{A.3.1}$$

Using $\frac{\partial}{\partial t} = \frac{c}{\sqrt{2}\xi} \frac{\partial}{\partial t'}$ and canceling common $\sqrt{\rho}$ factors, we get

$$i\hbar \frac{c}{\sqrt{2}\xi} \frac{\partial \psi'_{2D}}{\partial t'} = -\frac{\hbar^2}{2m} \frac{1}{\xi^2} \nabla'^2 \psi'_{2D} + g_{2D} \rho |\psi'_{2D}|^2 \psi'_{2D} + \chi_{2D} \xi^2 |\phi'_{2D}|^2 \psi'_{2D} - \mu_{2D} \psi'_{2D}.$$

Recalling $\mu = g_{2D} \rho$ and $\xi^2 = \frac{\hbar^2}{2m\mu}$, we further simplify to:

$$\begin{aligned}
i\hbar \frac{\partial \psi'_{2D}}{\partial t'} \frac{\sqrt{\mu/m}}{\sqrt{2}} \frac{\sqrt{2m\mu}}{\hbar} &= -\frac{\hbar^2}{2m} \frac{2m\mu}{\hbar^2} \nabla'^2 \psi'_{2D} \\
&+ \mu |\psi'_{2D}|^2 \psi'_{2D} \\
&+ \chi_{2D} \frac{\hbar^2}{2m\mu} |\phi'_{2D}|^2 \psi'_{2D} \\
&- \mu_{2D} \psi'_{2D}.
\end{aligned} \tag{A.3.2}$$

After canceling factors and dividing by μ , we arrive at

$$i \frac{\partial \psi'_{2D}}{\partial t'} = -\nabla'^2 \psi'_{2D} + |\psi'_{2D}|^2 \psi'_{2D} + \kappa |\phi'_{2D}|^2 \psi'_{2D} - \psi'_{2D},$$

where

$$\kappa = \frac{2m\chi_{2D}}{\hbar^2}.$$

Similarly, for the impurity equation, set $\phi_{2D} = \xi \phi'_{2D}$. Substituting in

$$i\hbar \frac{\partial \phi_{2D}}{\partial t} = -\frac{\hbar^2}{2m_i} \nabla_{2D}^2 \phi_{2D} + \chi_{2D} |\psi_{2D}|^2 \phi_{2D} - E_{2D} \phi_{2D},$$

and again using $\frac{\partial}{\partial t} = \frac{c}{\sqrt{2}\xi} \frac{\partial}{\partial t'}$, we arrive at

$$i \mu \frac{\partial \phi'_{2D}}{\partial t'} = - \frac{\hbar^2}{2m_i} \frac{2m \mu}{\hbar^2} \nabla'^2 \phi'_{2D} + \chi_{2D} \rho |\psi'_{2D}|^2 \phi'_{2D} - E_{2D} \phi'_{2D},$$

which simplifies to

$$i \mu \frac{\partial \phi'_{2D}}{\partial t'} = - \frac{m}{m_i} \mu \nabla'^2 \phi'_{2D} + \chi_{2D} \rho |\psi'_{2D}|^2 \phi'_{2D} - E_{2D} \phi'_{2D}.$$

Dividing by μ ,

$$i \frac{\partial \phi'_{2D}}{\partial t'} = - \frac{m}{m_i} \nabla'^2 \phi'_{2D} + \chi_{2D} \frac{\rho}{\mu} |\psi'_{2D}|^2 \phi'_{2D} - \frac{E_{2D}}{\mu} \phi'_{2D}.$$

Using $\mu = g_{2D} \rho$ and $\xi^2 = \frac{\hbar^2}{2m\mu}$, we rewrite

$$i \frac{\partial \phi'_{2D}}{\partial t'} = - \frac{m}{m_i} \nabla'^2 \phi'_{2D} + \frac{\chi_{2D}}{g_{2D}} |\psi'_{2D}|^2 \phi'_{2D} - \frac{2m\xi^2}{\hbar^2} E_{2D} \phi'_{2D}.$$

Multiplying by $\frac{m_i}{m}$, we obtain

$$i \tau \frac{\partial \phi'_{2D}}{\partial t'} = - \nabla'^2 \phi'_{2D} + \nu |\psi'_{2D}|^2 \phi'_{2D} - E'_{2D} \phi'_{2D},$$

where

$$\tau = \frac{m_i}{m}, \quad \nu = \frac{m_i \chi_{2D}}{m g_{2D}}, \quad E'_{2D} = \frac{2m_i \xi^2}{\hbar^2} E_{2D}.$$

Hence, in these dimensionless variables, the BEC and impurity equations have simpler forms that are more convenient for numerical and analytical investigations.

Bibliography

- [1] Barnabás Apagyi and Dániel Schumayer. Assessment of interspecies scattering lengths and stability of two-component Bose–Einstein condensates. *The European Physical Journal B-Condensed Matter and Complex Systems*, 45:55–61, 2005.
- [2] W. Bao and Q. Du. Computing the ground state solution of Bose–Einstein condensates by a normalized gradient flow. *SIAM Journal on Scientific Computing*, 25(5):1674–1697, 2004.
- [3] Weizhu Bao and Weijun Tang. Ground-state solution of Bose–Einstein condensate by directly minimizing the energy functional. *Journal of Computational Physics*, 187(1):230–254, 2003.
- [4] Natalia G Berloff. Padé approximations of solitary wave solutions of the Gross–Pitaevskii equation. *Journal of Physics A: Mathematical and General*, 37(5):1617, 2004.
- [5] P. B. Blakie and J. V. Porto. Adiabatic loading of bosons into optical lattices. *Physical Review A*, 69:013603, 2004.
- [6] Ashton S Bradley and Brian P Anderson. Energy spectra of vortex distributions in two-dimensional quantum turbulence. *Physical Review X*, 2(4):041001, 2012.
- [7] João EH Braz and Hugo Terças. Bound-state spectrum of an impurity in a quantum vortex. *Physical Review A*, 101(2):023607, 2020.

- [8] T. Byrnes, D. Rosseau, M. Khosla, A. Pyrkov, A. Thomasen, T. Mukai, S. Koyama, A. Abdelrahman, and E. O. Ilo-Okeke. Macroscopic quantum information processing using spin coherent states. *Optics Communications*, 337:102–113, 2015.
- [9] Tim Byrnes and Ebubechukwu O Ilo-Okeke. *Quantum atom optics: Theory and applications to quantum technology*. Cambridge university press, 2021.
- [10] J. Catani, G. Lamporesi, D. Naik, M. Gring, M. Inguscio, F. Minardi, A. Kantian, and T. Giamarchi. Quantum dynamics of impurities in a one-dimensional Bose gas. *Physical Review A*, 85:023623, 2012.
- [11] Jacopo Catani, Gabriele Lamporesi, Devashish Naik, Markus Gring, Massimo Inguscio, Federico Minardi, Adrian Kantian, and Thierry Giamarchi. Quantum dynamics of impurities in a one-dimensional Bose gas. *Physical Review A*, 85(2):023623, 2012.
- [12] Maria Luisa Chiofalo, Sauro Succi, and MP Tosi. Ground state of trapped interacting Bose-Einstein condensates by an explicit imaginary-time algorithm. *Physical Review E*, 62(5):7438, 2000.
- [13] S. P. Cockburn, A. Negretti, N. P. Proukakis, and C. Henkel. A comparison between microscopic methods for finite temperature Bose gases. *Physical Review A*, 83:043619, 2011.
- [14] E. A. Cornell and C. E. Wieman. Bose-Einstein condensation in a dilute gas: The first 70 years and some recent experiments. *Reviews of Modern Physics*, 74(3):875–893, 2002.
- [15] E. A. Cornell and C. E. Wieman. Vortices in a Bose-Einstein condensate. *Reviews of Modern Physics*, 74:875, 2002.
- [16] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari. Theory of Bose-Einstein condensation in trapped gases. *Rev. Mod. Phys.*, 71(3):463–512, 1999.

-
- [17] Matthew Edmonds, Minoru Eto, and Muneto Nitta. Synthetic superfluid chemistry with vortex-trapped quantum impurities. *Physical Review Research*, 3(2):023085, 2021.
- [18] MD Feit, JA Fleck Jr, and A Steiger. Solution of the Schrödinger equation by a spectral method. *Journal of Computational Physics*, 47(3):412–433, 1982.
- [19] A. L. Fetter. Rotating trapped Bose–Einstein condensates. *Rev. Mod. Phys.*, 81(2):647–691, 2009.
- [20] Alexander L Fetter. Vortices in an imperfect Bose gas. iv. translational velocity. *Physical Review*, 151(1):100, 1966.
- [21] Umberto Giuriato. *Dynamics of active particles in superfluids and their interaction with quantum vortices*. PhD thesis, Université Côte d’Azur, 2020.
- [22] A Görlitz, JM Vogels, AE Leanhardt, C Raman, TL Gustavson, JR Abo-Shaeer, AP Chikkatur, S Gupta, S Inouye, T Rosenband, et al. Realization of Bose-Einstein condensates in lower dimensions. *Physical review letters*, 87(13):130402, 2001.
- [23] A. Griffin, G. W. Stagg, N. P. Proukakis, and C. F. Barenghi. Vortex scattering by impurities in a Bose–Einstein condensate. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 50(11):115003, 2017.
- [24] David J. Griffiths. *Introduction to Quantum Mechanics*. Pearson Prentice Hall, 3rd edition, 2018.
- [25] F. Grusdt and E. Demler. New theoretical approaches to Bose polarons. arXiv preprint arXiv:1510.04934, 2015.
- [26] Emmanuel Mercado Gutierrez, Gustavo Alves de Oliveira, Kilvia Mayre Farias, Vanderlei Salvador Bagnato, and Patricia Christina Marques Castilho. Miscibility regimes in a ^{23}Na – ^{39}K quantum mixture. *Applied Sciences*, 11(19):9099, 2021.

- [27] Zoran Hadzibabic, Peter Krüger, Marc Cheneau, Baptiste Battelier, and Jean Dalibard. Berezinskii–Kosterlitz–Thouless crossover in a trapped atomic gas. *Nature*, 441(7097):1118–1121, 2006.
- [28] M.-G. Hu, M. J. Van de Graaff, D. Kedar, J. P. Corson, E. A. Cornell, and D. S. Jin. Bose polarons in the strongly interacting regime. *Physical Review Letters*, 117:055301, 2016.
- [29] J. A. M. Huhtamäki, M. Möttönen, T. Isoshima, V. Pietilä, and S. M. M. Virtanen. Splitting times of doubly quantized vortices in dilute Bose–Einstein condensates. *Physical Review Letters*, 97:110406, 2006.
- [30] A. D. Jackson, G. M. Kavoulakis, and C. J. Pethick. Effective quantum field theory of a Bose–Einstein condensate. *Physical Review A*, 58:2417, 1998.
- [31] B. Jackson, J. F. McCann, and C. S. Adams. Vortex formation in dilute inhomogeneous Bose–Einstein condensates. *Physical Review Letters*, 80(18):3903–3906, 1998.
- [32] Juha Javanainen and Janne Ruostekoski. Symbolic calculation in development of algorithms: split-step methods for the Gross–Pitaevskii equation. *Journal of Physics A: Mathematical and General*, 39(12):L179, 2006.
- [33] N. B. Jørgensen, L. Wacker, K. T. Skalmstang, M. M. Parish, J. Levinsen, R. S. Christensen, G. M. Bruun, and J. J. Arlt. Observation of attractive and repulsive polarons in a Bose–Einstein condensate. *Physical Review Letters*, 117:055302, 2016.
- [34] R. M. Kalas and D. Blume. Interaction-induced localization of an impurity in a trapped Bose–Einstein condensate. *Physical Review A*, 73:043608, 2006.
- [35] AM Kamchatnov. Expansion of Bose-Einstein condensates in lower dimensions. *arXiv preprint cond-mat/0310550*, 2003.
- [36] W. Ketterle. When atoms behave as waves: Bose–Einstein condensation and the atom laser. *Reviews of Modern Physics*, 74(4):1131–1151, 2002.

-
- [37] L. Landau. Theory of the superfluidity of helium ii. *Physical Review*, 60:356–358, 1941.
- [38] A. J. Leggett. Bose-Einstein condensation in the alkali gases: Some fundamental concepts. *Reviews of Modern Physics*, 73(2):307–356, 2001.
- [39] F Lingua, Luca Lepori, F Minardi, V Penna, and L Salasnich. Collision of impurities with Bose–Einstein condensates. *New Journal of Physics*, 20(4):045001, 2018.
- [40] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard. Vortex formation in a stirred Bose–Einstein condensate. *Physical Review Letters*, 84(5):806–809, 2000.
- [41] M. R. Matthews et al. Vortices in a Bose–Einstein condensate. *Physical Review Letters*, 83(13):2498–2501, 1999.
- [42] M. Möttönen, V. Pietilä, S. M. M. Virtanen, and M. M. Salomaa. Splitting of a doubly quantized vortex in a Bose–Einstein condensate. *Physical Review A*, 68:023611, 2003.
- [43] S. Palzer, C. Zipkes, C. Sias, and M. Köhl. Quantum transport through a tonks–girardeau gas. *Physical Review Letters*, 103:150601, 2009.
- [44] Sam Patrick, August Geelmuyden, Sebastian Erne, Carlo F Barenghi, and Silke Weinfurtner. Origin and evolution of the multiply quantized vortex instability. *Physical Review Research*, 4(4):043104, 2022.
- [45] Sam Patrick, August Geelmuyden, Sebastian Erne, Carlo F Barenghi, and Silke Weinfurtner. Quantum vortex instability and black hole superradiance. *Physical Review Research*, 4(3):033117, 2022.
- [46] C. J. Pethick and H. Smith. *Bose–Einstein Condensation in Dilute Gases*. Cambridge University Press, Cambridge, 2 edition, 2008.
- [47] L. P. Pitaevskii and S. Stringari. *Bose-Einstein Condensation and Superfluidity*. Oxford University Press, Oxford, 2016.

- [48] S. Rica and B. Roberts. Induced interaction and crystallization of self-localized impurity fields in a Bose–Einstein condensate. *Physical Review A*, 80:013609, 2009.
- [49] A. Richaud, G. Lamporesi, M. Capone, and A. Recati. Mass-driven vortex collisions in flat superfluids. *Physical Review A*, 107(5):053317, 2023.
- [50] G. Roati, C. D’Errico, L. Fallani, M. Fattori, C. Fort, M. Zaccanti, G. Modugno, M. Modugno, and M. Inguscio. Anderson localization of a non-interacting Bose–Einstein condensate. *Nature*, 453:895–898, 2008.
- [51] P. H. Roberts and N. G. Berloff. The nonlinear Schrödinger equation as a model of superfluidity. In R. J. Donnelly, C. F. Barenghi, and Y. A. Sergeev, editors, *Quantized Vortex Dynamics and Superfluid Turbulence*, volume 571 of *Lecture Notes in Physics*, pages 235–257. Springer, Berlin, 2001.
- [52] P. H. Roberts and N. G. Berloff. Vortex dynamics in trapped Bose–Einstein condensates. *Physics Letters A*, 289(1–2):61–65, 2001.
- [53] Jesus Rogel-Salazar. The Gross-Pitaevskii equation and bose–einstein condensates. *European Journal of Physics*, 34(2):247, 2013.
- [54] SJ Rooney, PB Blakie, BP Anderson, and AS Bradley. Suppression of kelvon-induced decay of quantized vortices in oblate Bose–Einstein condensates. *Physical Review A—Atomic, Molecular, and Optical Physics*, 84(2):023637, 2011.
- [55] 1PA Ruprecht, MJ Holland, Keith Burnett, and Mark Edwards. Time-dependent solution of the nonlinear Schrödinger equation for Bose-condensed trapped neutral atoms. *Physical Review A*, 51(6):4704, 1995.
- [56] J. J. Sakurai and Jim Napolitano. *Modern Quantum Mechanics*. Cambridge University Press, 2nd edition, 2021.
- [57] R. Scelle, T. Rentrop, A. Trautmann, T. Schuster, and M. K. Oberthaler. Motional coherence of fermions immersed in a Bose gas. *Physical Review Letters*, 111:070401, 2013.

- [58] Florian Schäfer, Naoto Mizukami, Phelan Yu, Shun Koibuchi, Adrien Bouscal, and Yoshiro Takahashi. Experimental realization of ultracold Yb-Li 7 mixtures in mixed dimensions. *Physical Review A*, 98(5):051602, 2018.
- [59] R. Shankar. *Principles of Quantum Mechanics*. Springer, 2nd edition, 1994.
- [60] Y. Shin, M. Saba, M. Vengalattore, T. A. Pasquini, C. Sanner, A. E. Leanhardt, M. Prentiss, D. E. Pritchard, and W. Ketterle. Dynamical instability of a doubly quantized vortex in a Bose–Einstein condensate. *Physical Review Letters*, 93:160406, 2004.
- [61] N. Spethmann, F. Kindermann, S. John, C. Weber, D. Meschede, and A. Widera. Dynamics of single neutral impurity atoms immersed in an ultracold gas. *Physical Review Letters*, 109:235301, 2012.
- [62] Jos Thijssen. *Computational physics*. Cambridge University Press, 2007.
- [63] L. A. Toikka and J. Brand. Exactly solvable model for a solitonic vortex in a compressible superfluid, 2017.
- [64] Alberto Villois. *Dynamics of Quantized Vortices and Electron Bubbles in the Gross-Pitaevskii Model of a Superfluid*. PhD thesis, University of East Anglia, 2018.
- [65] Alberto Villois, Giorgio Krstulovic, Davide Proment, and Hayder Salman. A vortex filament tracking method for the Gross–Pitaevskii model of a superfluid. *Journal of Physics A: Mathematical and Theoretical*, 49(41):415502, 2016.
- [66] Alberto Villois and Hayder Salman. Vortex nucleation limited mobility of free electron bubbles in the Gross-Pitaevskii model of a superfluid. *Physical Review B*, 97(9):094507, 2018.
- [67] T. Winiecki, B. Jackson, J. F. McCann, and C. S. Adams. Vortex shedding and drag in dilute Bose–Einstein condensates. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 33:4069–4088, 2000.

-
- [68] K Khani, G Del Pace, N Grani, D Hernández-Rajkov, B Donelli, G Roati, and L Pezzè. Tuning the critical current in toroidal superfluids via controllable impurities. *arXiv preprint arXiv:2511.10493*, 2025.